On the description and identifiability analysis of experiments with mixtures

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Abstract: Mixture designs are represented as sets of homogeneous polynomials. Techniques from computational commutative algebra are employed to deduce generalised confounding relationships on power products and to determine families of identifiable models.

Key words and phrases: Mixture designs, cone of a mixture design, fan of a design.

1 Introduction

In a mixture experiment the response variables depend on the proportion of the components or factors but not on the absolute amount of the mixture. There is a vast literature on experiments with mixtures, ranging from the seminal work by H. Scheffé Scheffé (1958, 1963) up to the work on optimal designs for second order mixture experiments by Zhang *et al.* Zhang et al. (2005). A textbook at its third edition is by J. Cornell Cornell (2002) and we refer the reader to the bibliographical list therein. See also Aitchison (1986).

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We study mixture designs with tools from computational commutative algebra (CCA). Specifically we tailor the polynomial algebra approach to identifiability analysis introduced in Pistone and Wynn (1996) to mixture designs. In a few words that approach consists of representing a design with a set of polynomials in k indeterminates, where k is the total number of factors in the design. Relevant statistical information and objects are retrieved by analysis of that polynomial set. From a practical view point, it is particularly useful in the analysis of non-regular designs by describing the set of polynomials which take the same values over all design points, and determining a finite generator set, called *generalised confounding relations*, and by determining classes of saturated hierarchical models identified by the design Caboara et al. (1999); Caboara and Riccomagno (1998); Giglio et al. (2001); Holliday et al. (1999); Pistone et al. (2000, 2001). A technical advantage of the algebraic statistic framework is the avoidance of the computation of the rank of design/model matrix which can be numerically ill conditioned.

The approach is computational and the algorithms provided e.g. in Pistone and Wynn (1996); Pistone et al. (2001) apply to mixture experiments. But the main results are in $k-1$ factors. In particular only slack models are obtained and all but one of the basic generalised confounding relations exclude entirely a factor. The one that involves all factors is a polynomial corresponding to the sum to one condition. In Giglio et al. (2001) the missing factor is reintroduced by homogenization. This might not be fully satisfactory, see Example 7. This asymmetry is intrinsic to the computational technology behind the mentioned algorithms, as they depend on a technical algebraic tool called a term ordering, see Appendix 8.1. In Holliday et al. (1999) this has been used at the advantage of the statistical analysis of a complex data set. Here we suggest to represent a mixture design not as *the set of all polynomials whose zeros include the design points* but as the subset of all *homogeneous* polynomials whose zeros include the design points. The first set is called the *design ideal* in Pistone et al. (2001); Pistone and Wynn (1996) and we call the second one the *cone ideal.* The use of the cone ideal reduces the effect of the aforementioned asymmetry, gives a natural representation of a compositional dataset as a set of polynomials, and retains the advantages, both computational and mathematical, of the use of algebraic statistics. The needed algorithms are suitably modified.

Our argument is based on three observations, already present in the literature in different forms. First, a mixture design is a projective object. Each point of the original mixture can be assimilated to a line through the point and the origin, excluding the origin itself. We call the set of all such lines the design cone. From an algebra geometric perspective this leads naturally to consideration of homogeneous polynomials and thus homogeneous type regression models. A reference to mixture models based on homogeneous polynomials is Draper and Pukelsheim (1998), where the mathematical tool employed is the Kronecker product. So homogeneous polynomials are at the base of our second observation. The third one is that no non-trivial polynomial function can be defined over a cone and rational polynomial models play a relevant role. Cornell Cornell (2002) collects and comments on many models for mixture experiments including ratios of polynomial models.

We shall make heavy use of CCA. In Appendix 8 we collect definitions and results from CCA we use, while in the main text we report only few essential ones. For an algebraic statistics neophyte it might be useful to read Appendix 8 first. There are many good books of computational commutative algebra, each with its peculiarities. We mainly use the undergraduate texts Cox et al. (1997) and Cox et al. (2004). Good books are also Adams and Loustaunau (1994) and Kreuzer and Robbiano (2000). We would like to put the reader in the condition to be able to perform the computations we present here for his/her own mixture designs. To this aim we specify the name of the commands and macros required in the syntax of CoCoA which is a freely available system for computing with multivariate polynomials CoCoATeam. We could have used other excellent and free softwares like *Singular* Greuel et al. (2005) or *Macaulay2* Grayson and Stillman. The proofs of the results we present are collected in Appendix 8 as exemplificative of the way geometric properties of the experimental plan are used.

In this paper we use the terms "interaction" to mean a monomial of total degree larger than one and "main effect" for monomials of degree one. For proper use of the terminology, statistical interpretation and analysis of the presence or absence of an interaction in the obtained model when dealing mixture experiments, we refer to the caveats, comments and solutions proposed in Claringbold (1955); Cornell (2002); Cox (1971); Piepel et al. (2002); Waller (1985).

In Section 2 we study the cone ideal and its link with the design ideal. We choose mixture experiments with n distinct points. In Section 3 we see a method to retrieve supports for homogeneous regression models identified by a mixture experiment. The algorithm in Section 3.1, which allows us to substitute some terms of the obtained model support retaining identifiability, strongly resembles the algebraic FGLM and Gröbner walk algorithms Faugère et al. (1993)(Cox et al., 2004, Ch.8§5). It proved to be very useful in practice. Some typical model structures from the literature are considered in Section 3.2. Practical examples are collected in Section 4 where the theoretical results of the paper are applied to simplex lattice designs, simplex centroid designs and axial designs. A brief exemplifying analysis of two data sets is performed.

2 The cone of a mixture design

The design space of a mixture design in k factors, $\mathcal{D} \subset \mathbb{R}^k$, is a regular $(k-1)$-dimensional simplex. For this reason we can see $\mathcal{D}$ alternatively in the affine space $\mathbb{R}^k$ or in the projective space $\mathbb{P}^{k-1}(\mathbb{R})$, where every point is associated to a line through the origin. We recall that $\mathbb{P}^{k-1}(\mathbb{R})$ is defined as the set of equivalence classes of points in $\mathbb{R}^k$ where p_1 and p_2 are equivalent if p_1, p_2 and $0 = (0, \ldots, 0) \in \mathbb{R}^k$ lie on the same line. Moreover, if $p \in \mathbb{P}^{k-1}(\mathbb{R})$ and $(x_1, \ldots, x_k) \in p$ then $(x_1 : \ldots : x_k)$ are the homogeneous coordinates of p and they are defined up to a multiple scalar. This leads us to identify naturally and uniquely $\mathcal{D}$ with the affine cone, $\mathcal{C}_{\mathcal{D}} \subset \mathbb{R}^k$, passing through the origin and $\mathcal{D}$: $\mathcal{C}_{\mathcal{D}} = \{\alpha d : d \in \mathcal{D} \text{ and } \alpha \in \mathbb{R}\} \subset \mathbb{R}^k$.

Example 1 The cone of $\mathcal{D}_1 = \{(0,1),\ (1,0),\ (1/2,1/2)\} \subset \mathbb{R}^2$ is $\mathcal{C}_{\mathcal{D}_1} = \{(0,a), (b,0), (c,c) : a, b, c, \in \mathbb{R}\} \subset \mathbb{R}^2$, to which we can associate three projective points. For example $(0,1), (1,0), (1,1) \in \mathbb{P}^1(\mathbb{R})$ are representative of the points in $\mathcal{D}_1$ as well.

An analogous construction of $\mathcal{C}_{\mathcal{D}_2}$ for $\mathcal{D}_2 = \{(0,0,1),\ (0,1,0),\ (1,0,0),\ (0,1/2,1/2),\ (1/2,0,1/2),\ (1/2,1/2,0),\ (1/3,1/3,1/3)\} \subset \mathbb{R}^3$ shows that in the projective space $\mathcal{D}_2$ can be represented in $\mathbb{P}^2(\mathbb{R})$ by a $2^3 \setminus \{(0,0,0)\}$ structure with levels $0, 1$: a fact we shall exploit in Section 4.

In order to define the design ideal and the cone ideal, let $\mathbb{R}[x_1, \ldots, x_k]$ be the set of all polynomials in $x_1, \ldots, x_k$ indeterminates and with real coefficients. A subset $I \subset \mathbb{R}[x_1, \ldots, x_k]$

is a *(polynomial) ideal* if $f+g \in I$ and $hf \in I$ for all $f, g \in I$ and $h \in \mathbb{R}[x_1, \ldots, x_k]$. The Hilbert basis theorem states that every polynomial ideal is finitely generated, where $G = \{g_1, \ldots, g_q\} \in \mathbb{R}[x_1, \ldots, x_k]$ generates I if for all $f \in I$ there exist $s_1, \ldots, s_q \in \mathbb{R}[x_1, \ldots, x_k]$ such that $f = \sum_{i=1}^{q} s_i g_i$. We write $I = \langle g_1, \ldots, g_q \rangle$. There exist special generating sets called Gröbner bases which depend on a term-ordering (see Appendix 8.1). The computation of a Gröbner basis from a generating set is considered here an "elementary" operation.

Definition 1 *For $\mathcal{D} \subset \mathbb{R}^k$ with n distinct points, define* $\text{Ideal}(\mathcal{D}) = \{f \in \mathbb{R}[x_1, \ldots, x_k] : f(d) = 0$ *for all* $d \in \mathcal{D}\}$.

Ideal($\mathcal{D}$) is a polynomial ideal Pistone et al. (2001); Pistone and Wynn (1996).

Example 2 $\text{Ideal}(\mathcal{D}_1) = \{s_1(x_1 + x_2 - 1) + s_2 x_1(x_1 - 1/2)(x_1 - 1) : s_1, s_2 \in \mathbb{R}[x_1, x_2]\}$ and $x_1 + x_2 - 1$ and $x_1(x_1 - 1/2)(x_1 - 1)$ form a generator set of Ideal($\mathcal{D}_1$).

If $\mathcal{D}$ is a mixture experiment, then the polynomial $x_1 + \ldots + x_k - 1$ always vanishes on the design points and thus belongs to Ideal($\mathcal{D}$) Giglio et al. (2001); Pistone et al. (2000). If the design lies on a face of the simplex then there will be a set $A \subseteq \{1, \ldots, k\}$ for which $\sum_{i \in A} x_i - 1 \in \text{Ideal}(\mathcal{D})$. As we shall show in Section 3, this restricts unduly the class of regression models for $\mathcal{D}$ retrieved with the algebraic statistics methodology and we need a more general theory. The idea is to exploit the representation of a mixture design as a cone. This will have consequences on the structure of the regression models we can associate to $\mathcal{D}$, thus extending the general theory of modelling and confounding particularly useful for non-regular fractions of a design.

The notion of a polynomial vanishing on a projective point is rather delicate. Indeed, the polynomial $x_2 - x_3^2$ vanishes on $p = (1, 4, 2)$. The points p and $q = (2, 8, 4) = 2p$ are the same point of $\mathbb{P}^2(\mathbb{R})$, but $x_2 - x_3^2$ does not vanish in q. A way to overcome this problem is to use only homogeneous polynomials. A polynomial is *homogeneous* if the total degree (sum of exponents) of each one of its terms (or power products) is the same. For example, $x_1 x_2 - x_3^2$ is a homogeneous polynomial of degree 2 which vanishes on $(\lambda, 4\lambda, 2\lambda)$ for all $\lambda \in \mathbb{R}$.

Definition 2 *The cone ideal of a mixture design is* $\mathrm{Ideal}(\mathcal{C}_\mathcal{D}) = \{f \in \mathbb{R}[x_1 \ldots, x_k] : f(d) = 0$ *for all* $d \in \mathcal{C}_\mathcal{D}\}$*, that is the ideal of polynomials vanishing on every point of the cone of the design.*

It is easy to show that $\mathrm{Ideal}(\mathcal{C}_\mathcal{D})$ is an ideal. Let $I, J \subset \mathbb{R}[x_1 \ldots, x_k]$ be two ideals generated by the sets G_I and G_J respectively. Then $I + J = \{f + g : f \in I \text{ and } g \in J\}$ is an ideal and $G_I \cup G_J$ is a generator set of $I + J$. A polynomial ideal is said to be *homogeneous* if for each $f \in I$ the homogeneous components of f are in I as well, equivalently if I admits a generator set formed by homogeneous polynomials (Cox et al., 1997, page 371). In some computer algebra packages macros are implemented to compute generator sets of $\mathrm{Ideal}(\mathcal{D})$ and $\mathrm{Ideal}(\mathcal{C}_\mathcal{D})$ directly from the coordinates of the points in $\mathcal{D}$. In CoCoA they are called `IdealOfPoints` and `IdealOfProjectivePoints`, respectively. See Abbott et al. (2000).

Theorem 1 *For a mixture design* $\mathcal{D}$

1. $\mathrm{Ideal}(\mathcal{C}_\mathcal{D}) = \langle f \in \mathbb{R}[x_1, \ldots, x_k] : f$ *is homogeneous and* $f(d) = 0$ *for all* $d \in \mathcal{D}\rangle$*, that is the largest homogeneous ideal in* $\mathbb{R}[x_1, \ldots, x_k]$ *vanishing on all the points of* $\mathcal{D}$*.*

2. $\mathrm{Ideal}(\mathcal{D}) = \mathrm{Ideal}(\mathcal{C}_\mathcal{D}) + \langle \sum_{i=1}^k x_i - 1\rangle$*, that is a polynomial vanishing on* $\mathcal{D}$ *can be written as combination of homogeneous components vanishing on* $\mathcal{D}$ *and the sum to one condition. If* G *is a generator set of* $\mathrm{Ideal}(\mathcal{C}_\mathcal{D})$ *then* G *and* $\sum_{i=1}^k x_i - 1$ *form a generator set of* $\mathrm{Ideal}(\mathcal{D})$*.*

Example 3 $\mathrm{Ideal}(\mathcal{C}_{\mathcal{D}_1}) = \langle x_1^2x_2 - x_1x_2^2\rangle$ and $\mathrm{Ideal}(\mathcal{C}_{\mathcal{D}_2}) = \langle x_1^2x_2 - x_1x_2^2, x_1^2x_3 - x_1x_3^2, x_3^2x_2 - x_3x_2^2\rangle$. For $\mathcal{D}_3 = \{(1,0,0), (0,1,0), (0,0,1), (1/3, 1/3, 1/3)\}$, $\mathrm{Ideal}(\mathcal{C}_{\mathcal{D}_3}) = \langle x_1x_3 - x_2x_3, x_1x_2 - x_2x_3\rangle$.

Theorem 1 states explicitly a method to construct a generating set of $\mathrm{Ideal}(\mathcal{D})$ from a generating set of $\mathrm{Ideal}(\mathcal{C}_\mathcal{D})$ by just adjoining the sum-to-one condition. Theorem 2 provides the converse. A term ordering is graded if $x^\alpha < x^\beta$ whenever $\sum_{i=1}^k \alpha_i < \sum_{i=1}^k \beta_i$. Gröbner bases (see Definition 5) are particular generator sets of a polynomial ideal, depend on a term ordering and are fundamental in the computations we need. Given a term ordering, a Gröbner basis is computed from a finite generator set of an ideal with the CoCoA command `GBasis`.

Theorem 2 *Let $\mathcal{D}$ be a mixture design and $\mathcal{C}_{\mathcal{D}}$ its cone. Let $G = \{l-1, g_1, \ldots, g_r\}$ be a Gröbner basis of* $\text{Ideal}(\mathcal{D})$ *with respect to a graded term ordering τ. Then $\{h(g_1), \ldots, h(g_r)\}$ is a generating set of* $\text{Ideal}(\mathcal{C}_{\mathcal{D}})$*, where $h(g)$ is the homogeneization of g with respect to $l = \sum_{i=1}^k x_i$.*

The generating set of the cone ideal obtained in Theorem 2 might not be a Gröbner basis because we do not control the leading term of $h(g_i)$ (see Definition 4 for leading term). The next example shows that if G is not a Gröbner basis the thesis of Theorem 2 might not hold.

Example 4 For $\mathcal{D} = \{(0,0,1), (0,1,0), (1,0,0), (1/2,1/2,0), (1/2,0,1/2), (0,1/2,1/2)\}$ $\text{Ideal}(\mathcal{D}) = \langle x_1+x_2+x_3-1, x_i(x_i-1/2)(x_i-1) : i = 1,2,3\rangle$ and the four listed polynomials form a generator set. For $l = x_1+x_2+x_3$ the ideal $I = \langle x_i(x_i-1/2l)(x_i-l) : i = 1,2,3\rangle \subsetneq \text{Ideal}(\mathcal{D})$ does not contain the polynomial $x_2^2x_3 - x_2x_3^2$, which instead belongs to $\text{Ideal}(\mathcal{D})$ and to $\text{Ideal}(\mathcal{C}_{\mathcal{D}})$. For a simple test to check ideal membership see Cox et al. (1997) and Pistone et al. (2001).

For $\alpha_i \in \mathbb{R}_{>0}$, $i = 0, \ldots, k$, $\text{Ideal}(\mathcal{C}_{\mathcal{D}}) + \langle \sum_{i=1}^k \alpha_i x_i - \alpha_0\rangle$ cuts the design cone not at the standard simplex. It returns another affine representative of the projective representation of the mixture experiment. In this case there is no immediate interpretation of the points on the hyperplane as a mixture experiment. An obvious interpretation is as a fraction of a bigger experiment with a linear generator.

2.1 Notes on confounding for mixture experiments

In Pistone and Wynn (1996) the authors use polynomials in $\text{Ideal}(\mathcal{D})$ to deduce (generalised) confounding relations between functions defined over a design $\mathcal{D}$. For example $x_1 + x_2 - 1 \in \text{Ideal}(\mathcal{D}_1)$ testifies that the polynomial functions x_1 and $1 - x_2$ take the same values over $\mathcal{D}_1$, likewise $x_1^2x_2 = x_1x_2^2$ over $\mathcal{D}_1$ because $x_1^2x_2 - x_1x_2^2 \in \text{Ideal}(\mathcal{D}_1)$. Indeed for all $d \in \mathcal{D}_1$, $(x_1^2x_2)(d) = (x_1x_2^2)(d) = 0$. In particular a Gröbner basis of $\text{Ideal}(\mathcal{D}_1)$ with respect to some term ordering gives a finite set of confounding relations which is sufficient to deduce all the others. Usually in classical experimental design theory this information is encoded in the alias table for the design, if it is defined.

The polynomial $\sum_i x_i - 1$ belongs to $\text{Ideal}(\mathcal{D})$ for every mixture design $\mathcal{D}$ Giglio et al. (2001); Pistone et al. (2000), thus confounding linear terms with the intercept. In particular the classical algebraic approach Pistone et al. (2001); Pistone and Wynn (1996) leads to the study of confounding relationships in a smaller set of factors and only when the sum-to-one condition is considered the remaining factors are reintroduced in the analysis.

Example 5 For the design $\mathcal{D}$ containing the corner points of the simplex in $\mathbb{R}^k$, for any corner point d and $\alpha \in \mathbb{Z}^k_{\geq 0}$

$$(x^\alpha)(d) = \begin{cases} 1 & \text{if } \alpha = (0,\dots,0) \\ (x_i)(d) & \text{if } \alpha = (0,\dots,\alpha_i,0,\dots,0) \\ 0 & \text{if at least two components of } \alpha \text{ are not zero} \end{cases}$$

Like $\operatorname{Ideal}(\mathcal{D})$ represents all generalised confounding relations over $\mathcal{D}$, a polynomial in $\operatorname{Ideal}(\mathcal{C}_\mathcal{D})$ expresses confounding among homogeneous components. In Section 4 we study some classes of mixture designs and discuss methods to construct classes of fractions by describing the generating polynomials of the cone of the fraction. That is by confounding some power products. We consider some symmetric mixture designs which have interesting statistical properties like equal variance estimates for main factors and for interaction terms where reasonable McConkey et al. (2000). They are considered to be particularly useful in the first stage of an experiment when the design region needs to be fairly screened.

3 Supports for regression models

In Pistone and Wynn (1996); Pistone et al. (2001) it is noted that for any design $\mathcal{D}$ the set of real functions over $\mathcal{D}$ is a $\mathbb{R}$-vector space and it is isomorphic to the coordinate ring $R[\mathcal{D}]$. In turn, $R[\mathcal{D}]$ is isomorphic to the quotient ring $\mathbb{R}[x_1,\dots,x_k]/\operatorname{Ideal}(\mathcal{D})$. The quotient space is a "computable algebraic object", for example using Gröbner bases. This makes it an important tool to discuss functions over a design.

For the definition and properties of a coordinate ring over a variety see (Cox et al., 1997, Ch.5), for $R[\mathcal{D}]$ see (Pistone et al., 2001, Ch.2§10,Ch.5) and Cox et al. (2004). See also Appendix 8.1. Here we only recall that the quotient ring $\mathbb{R}[x_1,\dots,x_k]/\operatorname{Ideal}(\mathcal{D})$ is the set of equivalence classes for the equivalence relationship $f \sim g$ if $f - g \in \operatorname{Ideal}(\mathcal{D})$. Special monomial $\mathbb{R}$-vector

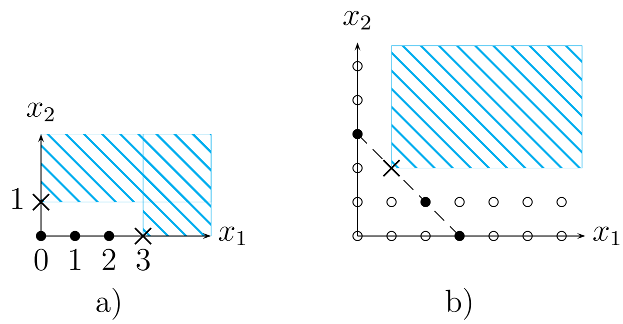

Figure 1: Standard monomials for Ideal($\mathcal{D}_1$) and Ideal($\mathcal{C}_{\mathcal{D}_1}$). Both cases were computed with a term order in which $x_2 > x_1$.

space bases of the quotient ring, called *standard monomials*, can be obtained from particular generating sets of Ideal($\mathcal{D}$), namely Gröbner bases and thus depend on a term ordering. The main steps of the computation are as follows.

1. Determine a Gröbner basis of Ideal($\mathcal{D}$) with respect to a term ordering, for example a Gröbner basis of Ideal($\mathcal{D}_1$) is $\{x_1^3 - 3/2x_1^2 + 1/2x_1, x_1 + x_2 - 1\}$ with respect to any term ordering for which $x_2 > x_1$;

2. compute the leading term of each element of the Gröbner basis, for the example x_1^3 and x_2;

3. determine all monomials which are not divisible by the leading terms, for the example 1, x_1 and x_1^2 (see Figure 1a).

The CoCoA macros `QuotientBasis` performs the algorithm above. Models returned in Step 3. above have a hierarchical structure in that if they include the monomial x^α then they also must include x^β for all $\beta \leq \alpha$ component-wise. A set of monomials with this property is called an order ideal. Order ideals can be used as support for saturated hierarchical polynomial models. The authors of McCullagh and Nelder (1989); Peixoto and Díaz (1996) among others strongly argue in favour of hierarchical regression models. Note that any standard monomial set includes the intercept. This might not be good when analysing a mixture experiment.

Indeed for a mixture experiment $\mathcal{D}$, the procedure above returns supports for slack models (Cornell, 2002, page 334). These can be homogenized to return the support for a homogeneous regression model Giglio et al. (2001). We could proceed differently and propose to adapt the above procedure to the homogeneous component of the design ideal, that is to work with the cone ideal instead of the design. The resulting homogeneous models can be different from those obtained by homogeneisation of a slack model as shown in Example 7.

There are two difficulties. First, $\mathbb{R}[x_1, \ldots, x_k]/\operatorname{Ideal}(\mathcal{C}_\mathcal{D})$ is infinite dimensional. Figure 1b) shows this for $\operatorname{Ideal}(\mathcal{C}_{\mathcal{D}_1})$. Second, usually a polynomial does not define a polynomial function on $\mathbb{P}^k(\mathbb{R})$ equivalently on $\mathcal{C}_\mathcal{D}$ (see the comment before Definition 2). One classical CCA remedy to address the first problem considers only monomials of a certain degree say $s \in \mathbb{Z}_{\geq 0}$. The basic algebraic definitions and results are in Appendices 8.2 and 8.4. Below we just apply them. For a mixture design $\mathcal{D}$

1. determine a Gröbner basis of $\operatorname{Ideal}(\mathcal{C}_\mathcal{D})$ with respect to a term ordering, for $\operatorname{Ideal}(\mathcal{C}_{\mathcal{D}_1})$ it is $\{x_1x_2^2 - x_1^2x_2\}$;

2. compute the leading terms of each element of the Gröbner basis, for the example $x_1x_2^2$ for term orderings for which $x_2 > x_1$;

3. consider all monomials of a sufficiently large total degree, for example in $\mathbb{R}[x_1, x_2]$ there are four monomials of degree $s = 3$, namely $x_1^3, x_1^2x_2, x_1x_2^2, x_2^3$;

4. determine all monomials of degree s not divisible by the leading terms of the Gröbner basis, in the example $x_1^3, x_1^2x_2, x_2^3$.

The monomials obtained in Step 4. above form a $\mathbb{R}$-vector space basis of the quotient space $\mathbb{R}[x_1, \ldots, x_k]_s/\operatorname{Ideal}(\mathcal{D})_s$ and form a subset of the set of standard monomials for the cone ideal. We call it the set of *degree s standard monomials*. As in the affine case it can be used to construct the support for regression models for $\mathcal{D}$. The correctness of this statement follows directly from Theorem 4 below.

Lemma 3 *Let $\mathcal{D}$ be a mixture design and $s \in \mathbb{Z}_{\geq 0}$ large enough. The $\mathbb{R}$-vector space $\mathbb{R}[x_1, \ldots, x_k]_{\leq s}/\,\mathrm{Ideal}(\mathcal{D})_{\leq s}$ has a basis $[g_1], \ldots, [g_n]$ where representatives of the equivalence classes can be chosen to be homogeneous of degree s.*

Theorem 4 *Let $\mathcal{D}$ be a mixture design. Then*

$$\dim \mathbb{R}[x_1, \ldots, x_k]_s/\mathrm{Ideal}(\mathcal{C}_{\mathcal{D}})_s = \dim \mathbb{R}[x_1, \ldots, x_k]_{\leq s}/\mathrm{Ideal}(\mathcal{D})_{\leq s}$$

If moreover $\mathcal{D}$ has n distinct points and s is sufficiently large then the dimensions equal n.

A monomial basis of degree s can be computed with the Singular macro `kbase`.

Example 6 The Gröbner basis of the homogeneous ideal of $\mathcal{D}_3 = \{(0,0,1), (0,1,0), (1,0,0), (1/3,1/3,1/3)\}$ and for any ordering for which $x_1 > x_2 > x_3$ is $\{x_1x_3 - x_2x_3, x_1x_2 - x_2x_3, x_2^2x_3 - x_2x_3^2\}$. The leading terms are x_1x_3, x_1x_2, $x_2^2x_3$ respectively. For $s = 3$ the standard monomials are $x_1^3, x_2^3, x_3^3, x_3^2x_2$: the largest possible number of terms we can identify with a four point design. For $s = 1$ we obtained the support for a non saturated model: x_1, x_2, x_3. Below we list the degree s standard monomials for all values of s.

s	list of monomials of degree s	degree s standard monomials
0	1	1
1	x_1, x_2, x_3	x_1, x_2, x_3
2	x_1^2, x_1x_2, x_2^2, x_1x_3, x_2x_3, x_3^2	x_1^2, x_2^2, x_2x_3, x_3^2
3	x_1^3, $x_1^2x_2$, $x_1x_2^2$, x_2^3, $x_1^2x_3$, $x_1x_2x_3$, $x_2^2x_3$, $x_1x_3^2$, $x_2x_3^2$, x_3^3	x_1^3, x_2^3, $x_2x_3^2$, x_3^3
$s > 3$	x_1^s, $x_1^{s-1}x_2$, $x_1^{s-2}x_2^2$, $\ldots$, x_3^s	x_1^s, x_2^s, $x_2x_3^{s-1}$, x_3^s

Example 7 The slack model obtained for $\mathcal{D}_3$ with respect to any ordering with $x_1 > x_2 > x_3$ has support $1, x_3, x_3^2, x_2$. By homogenising it following Giglio et al. (2001) we obtain $x_1^3, x_3x_1^2, x_3^2x_1, x_2x_1^2$, which is the support of a saturated homogeneous model of total degree 3 but different from the degree 3 model in Example 6. For slack models we consider "orthogonal" projection over the axis $x_k = 0$, while our procedure considers projection over the simplex.

Note the following things. *i)* For $s \geq n$ the procedure returns a degree s saturated support model. Example 6 shows that smaller values of s are possible, but the returned model support may not be saturated. *ii)* Equivalently for s large enough, the design/model matrix for $\mathcal{D}$ and the degree s standard monomials is invertible, and for any s it is full rank. *iii)* These standard monomials are not usually retrieved with the homogenization of a slack model, Example 7. *iv)* Different identifiable models can be obtained by varying the term ordering, as in the affine case. *v)* The degree s standard monomial set can be used as a starting set to obtain other types of identifiable sets as shown in Section 3.1.

3.1 Changing model

Often we want to substitute standard monomials in the set obtained with the methodology of Section 3, or in any other monomial basis of the quotient space, with monomials from a set δ that for some reason we would prefer to consider for the construction of the final regression model. The new set should still be a basis of the quotient space by $\operatorname{Ideal}(\mathcal{D})$. We present an algorithm to perform such substitution.

For a mixture design $\mathcal{D}$ let $\mathrm{SM}_{\tau,s}(\mathcal{C}_{\mathcal{D}})$ be the set of standard monomials of degree s with respect to a term ordering τ. We simplify the notation $\mathrm{SM}_{\tau,s}(\mathcal{C}_{\mathcal{D}})$ to SM_s. It seems reasonable to start with a monomial set of the same size as the design, thus we take s sufficiently large. Set $l = \sum_{i=1}^k x_i$ and let G be a Gröbner basis of $\operatorname{Ideal}(\mathcal{C}_{\mathcal{D}})$ with respect to τ.

Example 8 Our running example has $\mathcal{D} = \{(1/4, 1/4, 1/2),(1/8, 1/8, 3/4), (1/3, 1/3, 1/3), (1/5, 1/5, 3/5),(0, 0, 1)\}$, $s = 4$, τ is the default term ordering in CoCoA and $\delta = \{x_1, x_2, x_3, x_1x_2, x_1x_3, x_2x_3, x_1x_2x_3\}$ is a Scheffé type model (Scheffé, 1963, page 237), Scheffé (1958), (Cornell, 2002, page 334). Thus $\mathrm{SM}_s = \{x_2^4, x_2^3x_3, x_2^2x_3^2, x_2x_3^3, x_3^4\}$.

Step 0. $\eta := \mathrm{SM}_s$ is the current monomial basis of $\mathbb{R}[x_1, \ldots, x_k]/\operatorname{Ideal}(\mathcal{D})$, $W := \emptyset$ set of rewriting rules, $\delta' := \delta$.

Step 1. Chose a monomial $w \in \delta'$ and let $\deg(w)$ be its total degree and update $\delta' := \delta' \setminus \{w\}$.

Compute the normal form of $wl^{s-\deg(w)}$ with respect to G

$$\begin{aligned}\mathrm{NF}(wl^{s-\deg(w)}) &= \sum_{x^\alpha \in \mathrm{SM}_s} \theta_\alpha x^\alpha \qquad \text{for } \theta_\alpha \in \mathbb{R} \\ &= \sum_{x^\alpha \in \eta} \theta'_\alpha x^\alpha\end{aligned}$$

These equalities are valid over $\mathcal{D}$. The second one follows by substituting the rules in W where necessary (this can be cumbersome in practice).

Step 2. Chose a term x^β in $\sum_{x^\alpha \in \eta} \theta'_\alpha x^\alpha$ for which $\theta'_\beta \neq 0$ and $x^\beta \notin \delta$, equivalently $x^\beta \in \mathrm{SM}_s$. If there is not such β then repeat **Step 1.**

Step 3. Update $\eta := \eta \setminus \{x^\beta\} \cup \{w\}$. In each $g \in W$ substitute x^β with $\frac{1}{\theta'_\beta}(w - \sum_{x^\alpha \in \eta \setminus \{x^\beta\}} \theta'_\alpha x^\alpha)$ and get g'. Update $W = \{x^\beta \equiv \frac{1}{\theta'_\beta}(w - \sum_{x^\alpha \in \eta \setminus \{x^\beta\}} \theta'_\alpha x^\alpha), g' : g \in W\}$.

Step 4. Repeat from **Step 1.** until $\delta' = \emptyset$.

This is a variation of the algorithm in Babson et al. (2003) where the set δ is the union of all the stairs and their border sets. Stair is another name for an order ideal. The border of a monomial set is computed by multiplying any monomial in the set by x_i, in turn for $i = 1, \ldots, k$ and excluding monomials already in the set. The starting monomial set used in Babson et al. (2003), what we call η, is a stair as well. The correctness of the our algorithm is proved as for that in Babson et al. (2003). Its termination is guaranteed by the updating of δ' in Step 1. and the finiteness of δ. While in Babson et al. (2003) the algorithm terminates when η contains n monomials which are linearly independent and form an order ideal according to the chosen term ordering. In particular the algorithm in Babson et al. (2003) returns a support for a saturated hierarchical model. Different final monomial sets, and of possibly different sizes, might be obtained by choosing different monomials in Step 1. In the introduction we already mentioned the similarity with the algorithms in Faugère et al. (1993) and (Cox et al., 2004, Ch.8§5).

Example 9 For Example 8 the basic steps of the algorithm are as follows. **Step 1.** We chose terms in δ in the order they are presented left-to-right in Example 8. Thus $w = x_1$ of degree 1 and for $(x_1 + x_2 + x_3)^3 x_1$ $\mathrm{NF}(x_1 l^3) = 8x_2^4 + 12x_2^3 x_3 + 6x_2^2 x_3^2 + x_2 x_3^3$. We update

$\delta' = \delta' \setminus \{x_1\}$. **Steps 2. and 3.** We select $x^\beta = x_2^4$ and update $\eta = \{x_1, x_2^3x_3, x_2^2x_3^2, x_2x_3^3, x_3^4\}$ and $W = \{\ x_2^4 \equiv 1/8x_1 - 12/8x_2^3x_3 - 3/4x_2^2x_3^2 - 1/8x_2x_3^3\}$. **Steps 1. and 2.** Next $w = x_2$, update $\delta' = \delta' \setminus \{x_2\}$ and $\text{NF}(x_2l^3) = 8x_2^4 + 12x_2^3x_3 + 6x_2^2x_3^2 + x_2x_3^3 = x_1$. There is no element to select as, over $\mathcal{D}$, $x_1 = x_2$ which is already included in η. **Steps 1. to 3.** We try the next monomial in δ, $w = x_3$ which can replace $x_2^3x_3$. We update $\eta = \{x_1, x_3, x_2^2x_3^2, x_2x_3^3, x_3^4\}$, $W = W \cup \{x_2^3x_3 \equiv 1/8x_3 - 12/8x_2^2x_3^2 - 3/4x_2x_3^3 - x_3^4\}$ and δ'. **Steps 1. to 3.** We update η substituting $x_2^2x_3^2$ with x_1x_2 and add the rule $x_2^2x_3^2 \equiv x_1x_2 - x_2x_3^3 - 1/4x_3^4 - 1/2x_1 + 1/4x_3$ to W. **Steps 1. to 3.** Now we substitute in η the monomial $x_2x_3^3$ with x_1x_3 and add the rule $x_2x_3^3 \equiv -1/16x_3^4 + 4/9x_1x_2 + 2/9x_1x_2 - 2/9x_1 + 4/243x_3$ to W. The current η is $\{x_1, x_3, x_1x_2, x_1x_3, x_3^4\}$. **Steps 1. and 2.** The next candidate in δ is x_2x_3. However, there is no interchange possible as over $\mathcal{D}$, $x_2x_3 = x_1x_3$ and $x_1x_3 \in \eta$. At this step $\delta' = \{x_1x_2x_3\}$. **Steps 1. to 3.** The final monomial to be removed from η is x_3^4 which is substituted with $x_1x_2x_3$. We add the rule $x_3^4 \equiv 6x_1x_2x_3 + 14/3x_1x_2 - 11/3x_1x_3 - 7/3x_1 + 235/162x_3$. **Step 4.** As now $\delta' = \emptyset$, the algorithm ends with the new model/representatives of classes of the quotient space $\eta = \{x_1, x_3, x_1x_2, x_1x_3, x_1x_2x_3\}$ and with the updated set of rules W to express polynomials in terms of monomials in η.

The starting monomial set does not need to be a SM_s set but could be any other set of monomials which are linearly independent over $\mathcal{D}$. McConkey *et al.* (2000) McConkey et al. (2000) describe the confounding relationship between the parameters of the Scheffé quadratic model and the model with support x_i and $x_i(1 - x_i)$, $i = 1, \ldots, k$ used to describe the average deviation from linearity caused by an individual component on mixing with the other components. The set δ could then be this support and for $w = x_i(1-x_i)$ the normal form of $x_i \sum_{j \neq i} x_j$ is computed.

Example 10 For $\mathcal{D}_3$ a brother algorithm of the above can be summarised in the following table, which expresses the inverse of the rewriting rules in W, for $\delta = \{x_i, x_i(1 - x_i) : i = 1, 2, 3\}$,

$\text{SM}_\tau = \{1, x_2, x_3, x_3^2\}$ and any τ for which $x_1 > x_2 > x_3$

$$B = \begin{array}{r|cccc|} & 1 & x_2 & x_3 & x_3^2 \\ \hline x_1 & 1 & -1 & -1 & 0 \\ x_2 & 0 & 1 & 0 & 0 \\ x_3 & 0 & 0 & 1 & 0 \\ x_1(1-x_1) & 0 & 0 & 1 & -1 \\ x_2(1-x_2) & 0 & 0 & 1 & -1 \\ x_3(1-x_3) & 0 & 0 & 1 & -1 \\ \hline \end{array}$$

3.2 Rational models

Sets of linearly independent functions over $\mathcal{D}$ can be defined starting from a $\mathbb{R}$-vector space basis of $\mathbb{R}[x_1, \ldots, x_k]/\operatorname{Ideal}(\mathcal{D})$ and considering ratios of homogeneous polynomials of the same degree.

Example 11 To $\mathcal{D}_1$ and $\{x_1, x_2, x_1x_2\}$ we associate the real valued rational functions $f_1 = \frac{x_1}{x_1+x_2}$, $f_2 = \frac{x_2}{x_1+x_2}$, $f_3 = \frac{x_1x_2}{(x_1+x_2)^2}$ where for example

$$\begin{array}{rccc} \frac{x_1}{(x_1+x_2)}: & \mathcal{C}_{\mathcal{D}_1} & \longrightarrow & \mathbb{R} \\ & (0,1) & \longmapsto & 0 \\ & (1,0) & \longmapsto & 1 \\ & (1,1) & \longmapsto & 1/2 \end{array}$$

The design matrix of $\mathcal{D}_1$ and f_1, f_2, f_3 is the same as that of $\mathcal{D}_1$ and x_1, x_2, x_1x_2. As over $\mathcal{D}_1$ $x_1 + x_2 = 1$, there is no issue in considering a polynomial model as usually done. If $x_1 + x_2 = a$ for some $a \in \mathbb{R} \setminus \{0\}$ then a mixture-amount model either in polynomial form (Cornell, 2002, §7.9) or rational form can be considered. The natural rational model which includes terms like $\frac{x_1}{a}$ can be written as a polynomial model by introducing two extra indeterminates say $t = 1/a$ and the extra polynomial $ta - 1$. Namely, for $\theta_1, \theta_2, \theta_{11}$ parameters, $\theta_1 x_1 + \theta_2 x_2 + \theta_{11} x_1 x_2$ becomes the rational model $\theta_1 \frac{x_1}{(x_1+x_2)} + \theta_2 \frac{x_1}{(x_1+x_2)} + \theta_{11} \frac{x_1x_2}{(x_1+x_2)^2}$ which in turn translates into the pair of polynomials $at - 1$ and $\theta_1 x_1 + \theta_2 x_2 + \theta_{11} x_1 x_2 a$.

Sometimes in the literature x_i is substituted with $x_i/(1-x_i)$ for $i \in A \subseteq \{1,\ldots,k\}$. These functions are defined over $\mathcal{D}$ and not over $\mathcal{C}_\mathcal{D}$ and are used as screening models Cornell (2002). As the corner points with component 1 at the coordinates in A should not in the design, the normal forms (see Definition 6) of the polynomials $1-x_i$, $i \in A$, are not zero. The authors have not been able to prove of disprove the assertion that the linear independence of a set $\{x^\alpha\}$ implies the linear independence of the "normalised" $\{x^\alpha / \prod_{i=1}^k (1-x_i)^{\alpha_i}\}$ with $\alpha = (\alpha_1,\ldots,\alpha_k)$. An example is analysed in Section 5.2.

Some mixture model forms include inverse terms to model extreme changes in the response behaviour (see (Cornell, 2002, Ch.6)) for example

$$\sum_{i=1}^k \theta_i x_i + \sum_{i=1}^k \theta_{-i} x_i^{-1} \tag{1}$$

when no design point has a zero coordinate. Rather than checking that the design/model matrix is full rank we could employ a standard trick in algebra which allows us to transform the above in a polynomial model in two ways at least. Set $y_i = x_i^{-1}$, to $\mathrm{Ideal}(\mathcal{D})$ add the polynomials $y_i x_i - 1$, $i = 1\ldots,k$ and work in $\mathbb{R}[y_1,\ldots,y_k,x_1,\ldots,x_k]$ with a term ordering which eliminates the y_i indeterminates (Cox et al., 1997, page 72). Alternatively, rewrite Model (1) as $y\sum_{i=1}^k \theta_i x_i + \sum_{i=1}^k \theta_{-i} \prod_{j\neq i, j=1}^k x_j$ and add the polynomial $y\prod_{i=1}^k x_i - 1$.

3.3 Logistic transformations

Mixture designs in $\mathbb{R}^{k+1}$ with no point on the boundary are obtained from a full factorial designs in $\mathbb{R}^k$ by applying the additive logistic transformation or any other transformation that maps $\mathbb{R}^k$ into the interior of the simplex in one higher dimension. Let $\mathcal{F} \subset \mathbb{R}^k$ be a full factorial design with $l_{i1},\ldots,l_{in_i} \in \mathbb{R}$ levels for factor i. Then

$$\mathrm{Ideal}(\mathcal{F}) = \langle \prod_{j=1}^{n_i} (z_i - l_{ij}), \qquad i = 1,\ldots,k\rangle \subset \mathbb{R}[z_1,\ldots,z_k] \tag{2}$$

with the unique standard monomial set

$$\left\{ z^\alpha : \alpha \in \prod_{i=1}^k \{0,1,\ldots,n_i-1\} \right\} \tag{3}$$

The additive logistic transformation $x_i = \dfrac{e^{z_i}}{1+\sum_{j=1}^{k} e^{z_j}}$, for $i = 1, \ldots, k$ and $x_{k+1} = \dfrac{1}{1+\sum_{j=1}^{k} e^{z_j}}$ with inverse transformation

$$z_i \quad = \quad \ln \frac{x_i}{x_{k+1}} \quad i = 1, \ldots, k \tag{4}$$

maps $z = (z_1, \ldots, z_k) \in \mathcal{F}$ into a mixture point. Call $\mathcal{G}$ the collection of such mixture points. Note that substitution of the inverse relationship in (3) returns the support for a generalisation of the model (12.6) in Aitchison (1986).

Substitution of (4) in (2) and inclusion of the sum to one condition in the x_i space gives $\text{Ideal}(\mathcal{G}) = \langle \sum_{i=1}^{k+1} x_i - 1, \prod_{j=1}^{n_i} (x_i - x_{k+1} e^{l_{ij}}),\ i = 1, \ldots, k \rangle \subset \mathbb{R}[x_1, \ldots, x_{k+1}]$.

Direct application of the Buchberger algorithm (Cox et al., 1997, Ch.2§7) shows that the polynomials above form a Gröbner basis for any term ordering for which $x_{k+1} > x_i$ for all $i = 1, \ldots, k$. The corresponding standard monomial set is directly linked with the one of the full factorial in (3) and it gives the support for a slack model identified by $\mathcal{G}$

$$\{x_1^{\alpha_1} \cdots x_k^{\alpha_k} : \alpha_i \in \{0, 1, \ldots, n_i - 1\}, i = 1, \ldots, k\} \tag{5}$$

As another example of the simplicity and elegance of the algebraic statistics note that the recursive structure of the multiplicative logistic transformation $x_i = \dfrac{e^{z_i}}{\prod_{j=1}^{i} (1 + e^{z_j})}$ for $i = 1, \ldots, k$ $x_{k+1} = \dfrac{1}{\prod_{j=1}^{k} (1 + e^{z_j})}$ with inverse $z_i = \ln \dfrac{x_i}{1 - x_1 - \ldots - x_i}$, $i = 1, \ldots, k$ sending $\mathcal{F}$ into $\mathcal{H}$ is reflected in the recursive structure of the polynomials in

$$\text{Ideal}(\mathcal{H}) = \langle \sum_{i=1}^{k+1} x_i - 1, \prod_{j=1}^{n_i} \Big(x_i(1 + e^{l_{ij}}) - (1 - x_1 - \ldots - x_{i-1}) e^{l_{ij}} \Big) :\ i = 1, \ldots, k \rangle$$

There exists at least a term ordering for which the leading terms of the polynomials above are $x_i^{n_i}$ and for the sum to one condition it is x_{k+1}. The corresponding standard basis is again (5) while the substitution of the inverse relationship in (3) returns the support for a generalisation of the model (12.7) in Aitchison (1986).

4 Some symmetric mixture designs

We start by stating a simple fact valid for mixture designs including corner points, which is the algebraic representation of the well known fact that contrasts of all linear effects with the intercept are identifiable by such an experiment.

Lemma 5 *Let $\mathcal{D} \subset \mathbb{R}^k$ be the mixture design formed by the k corner points of the simplex and τ be a term order. If $x_k > x_i$ for all $i \in \{1, \ldots, k\}$, then the (generalised) confounding relationship for a general interaction $x_\alpha = x_1^{\alpha_1} \ldots x_k^{\alpha_k}$, $\alpha \in \mathbb{Z}^k_{\geq 0}$, is*

$$\mathrm{NF}(x^\alpha) = \begin{cases} 1 - \sum_{i=1}^{k-1} x_i & \text{if } x^\alpha = x_k^{\alpha_k} \\ x_i & \text{if } x^\alpha = x_i, i = 1, \ldots, k-1 \\ 0 & \text{if } \alpha \text{ has at least two non zero components} \\ 1 & \text{if } \alpha = (0, \ldots, 0). \end{cases} \tag{6}$$

Theorem 6 *Let $\mathcal{D}$ be a mixture that contains the corner points. Let τ be a graded term ordering for which $x_k > x_i$ for all i. Then*

1. *$1, x_1, \ldots, x_{k-1}$ are linearly independent monomials over $\mathcal{D}$,*
2. *the coefficient of the term 1 in $\mathrm{NF}(x_k^{\alpha_k})$ is 1,*
3. *the coefficient of the term 1 in $\mathrm{NF}(x^\alpha)$, with $x^\alpha \neq x_k^{\alpha_k}$ is 0.*

4.1 Simplex lattice designs

In Scheffé (1958) Scheffé discusses uniformly spaced distributions of points on the simplex to explore the whole factor space and calls them *simplex lattice designs*. A $\{k, m\}$ simplex lattice design is the intersection of the simplex in $\mathbb{R}^k$ and the full factorial design in k factors and with the $m + 1$ uniformly spaced levels $\{0, 1/m, \ldots, 1\}$. It has $\binom{m+k-1}{m}$ points. Directly from that description we deduce that for the $\{k, m\}$ simplex lattice design, $\mathcal{D}$, $\mathrm{Ideal}(\mathcal{D}) = \langle \prod_{j=0}^m (x_1 - j/m), \ldots, \prod_{j=0}^m (x_k - j/m), \sum_{i=1}^k x_i - 1 \rangle$ where the first k polynomials are a simple generating set of the full factorial design and the last one is the simplex condition.

The set of slack models identified by $\mathcal{D}$ are well classified and they are k as Theorem 7 shows. In Caboara et al. (1999) the set of order ideals identified by a design and obtained via the procedure in Section 3 is called the algebraic fan of the design.

$\mathcal{D}$	Ideal($\mathcal{C}_\mathcal{D}$)	Number of terms
$\{k,1\}$	Ideal($\mathcal{C}_\mathcal{D}$) $= \langle x_i x_j : i \neq j \rangle$	$\binom{k}{2}$
$\{k,2\}$	Ideal($\mathcal{C}_\mathcal{D}$) $= \langle x_i^2 x_j - x_i x_j^2, x_i x_j x_l : i \neq j \neq l \rangle$	$\binom{k}{2} + \binom{k}{3}$
$\{2,m\}$	Ideal($\mathcal{C}_\mathcal{D}$) $= \langle x_1 x_2 f(x_1, x_2) \rangle$	

Table 1: Ideal($\mathcal{C}_\mathcal{D}$) for some simplex lattice designs

Theorem 7 The algebraic fan of a $\{k, m\}$ simplex lattice design has size k. Each one of its elements is the set of all monomials up to degree m in $k-1$ factors.

Corollary 8 There are no other saturated hierarchical polynomial models identified by the $\{k, m\}$ simplex lattice design apart from those of Theorem 7.

By Theorem 1 Ideal($\mathcal{C}_\mathcal{D}$) is the radical of the ideal generated by the homogeneous polynomials $\prod_{j=0}^{m}(x_i - lj/m)$ for $i = 1, \ldots, k$, $l = \sum_{i=1}^{k} x_i$. Table 4.1 reports a Gröbner basis for Ideal($\mathcal{C}_\mathcal{D}$) for various combinations of k and m. It uses the following functions $g(x_1, x_2, w) = \prod_{j=1}^{w}(x_1 - \frac{jx_2}{m-j})(x_1 - x_2\frac{m-j}{j})$ for $w \in \mathbb{Z}_{>0}$

$$f(x_1, x_2) = \begin{cases} 1 & \text{if } m = 1 \\ g(x_1, x_2, w) & \text{if } m \text{ odd, } m \neq 1 \text{ and } w = \lfloor m/2 \rfloor \\ (x_1 - x_2) g(x_1, x_2, w) & \text{for } m \text{ even and } w = m/2 - 1 \end{cases}$$

Fractions of a $\{k, m\}$ design, or of any other design, can be built by confounding identifiable terms Pistone et al. (2001). A systematic use of the Hilbert function computes how many terms will be in any corresponding saturated model support and, in the homogeneous case, how many terms of each degree can be at most included. The relevant theory on Hilbert functions is in Appendix 8.4. In some cases the generator set of the fraction is easy enough to allow the determination of the actual design points by direct investigation.

Example 12 For the $\{4,4\}$ design, the binomials $x_1x_2 - x_3x_4$, $x_1x_3 - x_2x_4$ and $x_1x_4 - x_2x_3$ added to the generator set of the ideal of either the design or its cone, select the four corner points and the centroid point. They also establish that the terms in each binomial are confounded, take the same values over the selected fraction.

The polynomial $(x_1 - x_2)(x_3 - x_4)$ selects the 15 points for which $x_1 = x_2$ or $x_3 = x_4$, see Example 18. With respect to the default term ordering in CoCoA we obtain the support for a slack model $1, x_4, x_4^2, x_4^3, x_4^4, x_3, x_3^2, x_2, x_2^2, x_2^3, x_2^4, x_3x_4, x_3x_4^2, x_2x_4, x_2^2x_4$.

For the same fraction and term ordering, the support for a homogeneous model of total degree $s = 0, \dots, 4$ is

s	SM$_s$
0	1
1	x_1, x_2, x_3, x_4
2	$x_1^2, x_1x_2, x_2^2, x_2x_3, x_3^2, x_1x_4, x_2x_4, x_3x_4, x_4^2$
3	$x_1^3, x_1^2x_2, x_1x_2^2, x_2^3, x_2x_3^2, x_3^3, x_2^2x_4, x_2x_3x_4, x_3^2x_4, x_1x_4^2, x_2x_4^2, x_3x_4^2, x_4^3$
4	$x_1^4, x_1^3x_2, x_1^2x_2^2, x_1x_2^3, x_2^4, x_2x_3^3, x_3^4, x_3^3x_4, x_2^2x_4^2, x_2x_3x_4^2, x_3^2x_4^2, x_1x_4^3,$
	$x_2x_4^3, x_3x_4^3, x_4^4$

In Example 12 we had to take the saturation Hartshorne (1977) of the ideal generated by the homogeneous polynomials $\prod_{j=0}^{4}(x_i - lj/4)$, $i = 1,2,3,4$ and $(x_1 - x_2)(x_3 - x_4)$ with respect to x_1, x_2, x_3, x_4. The saturation is an algebraic operation which allows us to take the largest homogeneous ideal defined over a variety, namely the ideal of the variety. It can be performed in e.g. CoCoA with the command `Saturation`. We do not study it here any further and refer to Hartshorne (1977), but we add another example and some comments in order to clarify the algebraic motivation.

Example 13 In $\mathbb{P}^3$ with coordinates x, y, z, w consider the two skew lines $L_1 = \mathrm{V}(x, y)$ and $L_2 = \mathrm{V}(z, w)$ and the curve $C = L_1 \cup L_2$ whose ideal is $\mathrm{Ideal}(C) = \mathrm{Ideal}(L_1) \cap \mathrm{Ideal}(L_2) = \langle xz, xw, yz, yw \rangle$. If we cut C with the plane $H = \mathrm{V}(y+z)$ we obtain two points $A_1 = (0:0:0:1)$ and $A_2 = (1:0:0:0)$ whose ideal is $\mathrm{Ideal}(A_1, A_2) = \langle y, z, xw \rangle$. Of course it is natural to compute the ideal $J = \mathrm{Ideal}(C) + \mathrm{Ideal}(y+z)$ more than the coordinates of the intersection points, and we have $J = \langle y+z, xy, xw, y^2, yw \rangle$.

Clearly $J \neq \mathrm{Ideal}(A_1, A_2)$ and it is easy to verify that $J_s = \mathrm{Ideal}(A_1, A_2)_s$ for $s \geq 2$. So, we can say that the sum of the two ideals I and J is asymptotically equal to the ideal of the intersection of the varieties $\mathrm{V}(I)$ and $\mathrm{V}(J)$. In fact, when we compute combinations of homogeneous polynomials we get always polynomials of degree larger than or equal to the degree of the operands.

The algebraic operation that allows us to compute the ideal of $\mathrm{V}(I) \cap \mathrm{V}(J)$ from $I + J$ is the *saturation* with respect to the ideal generated by all the indeterminates, and it consists in looking for homogeneous polynomials f with the property that $f x_i^{m_i} \in I + J$ for some $m_i \in \mathbb{Z}_{>0}$ and for every $i = 1, \ldots, k$.

In the affine space this phenomenon does not show up because when computing combinations of non homogeneous polynomials we can obtain polynomials of degree strictly smaller than the degree of the operands.

4.2 Simplex centroid designs

Simplex centroid designs introduced in Scheffé (1963) are mixture designs in which coordinates are zero or equal to each other. Thus in the k dimensional simple centroid design there are k points of the form $(1, 0, \ldots, 0)$, $\binom{k}{2}$ of the form $(\frac{1}{2}, \frac{1}{2}, 0, \ldots, 0)$, $\binom{k}{3}$ of the form $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}, 0, \ldots, 0)$, ..., and the point $(\frac{1}{k}, \ldots, \frac{1}{k})$: a total of $\sum_{j=1}^{k} \binom{k}{j} = 2^k - 1$ points. This design is the projection of the full factorial design with levels 0 and 1, on the simplex in $\mathbb{R}^k$ with respect to the origin. Again easily we see that there are $2^k - 1$ points. We rename "2^k design" the full factorial design with levels 0 and 1 in k factors.

The ideal of the cone of $\mathcal{D}$ is $\mathrm{Ideal}(\mathcal{C}_{\mathcal{D}}) = \langle x_i^2 x_j - x_i x_j^2 : i, j = 1, \ldots, k; i \neq j \rangle$. The geometry of the design is easily deduced by inspection of the factorised generators $x_i x_j (x_i - x_j)$: coordinates of a point in $\mathcal{D}$ are either 0 or equal to each other. The generator set given for $\mathrm{Ideal}(\mathcal{C}_{\mathcal{D}})$ is a Gröbner basis with respect to any term ordering. The proof is a straightforward application of the S-polynomial test (Cox et al., 1997, Ch.2§6Th.6).

Also the construction of $\mathrm{Ideal}(\mathcal{D})$ can be based on the derivation of the simplex centroid design from the 2^k design but it is more complicated and involves techniques from elimination theory (Cox et al., 1997, Ch.3). We may want to do this when for some reasons we do not want to list the mixture point coordinates. The steps of the constructions are as follows.

1. The ideal of the 2^k design is $\langle x_i^2 - x_i : i = 1, \ldots, k\rangle$.

2. The origin can be removed by adjoining the polynomial given by the sum of the elementary symmetric polynomials and 1 with alternate signs (Cox et al., 1997, Ch.7§2). The elementary symmetric polynomials in $\mathbb{R}[x_1, \ldots, x_k]$ are $\sigma_1 = (x_1 + \ldots + x_k)$, …, $\sigma_r = (\sum_{i_1<i_2<\cdots<i_r} x_{i_1} \ldots x_{i_r})$, …, $\sigma_k = (x_1 \ldots x_k)$.

3. The simplicial projection is performed in two steps Bocci et al. (2005). Extend the polynomial ring with the variables $y_1, \ldots, y_k$ and adjoin to the ideal above the polynomials $y_i(\sum_{j=1}^k x_j) - x_i$.

4. Eliminate the indeterminates $x_i, i = 1, \ldots, k$ from the ideal obtained in 3. above (Cox et al., 1997, Ch.3) to get Ideal$(\mathcal{D})$ which is now expressed in the y_i indeterminates.

Example 14 For $k = 3$ the affine ideal of a 2^3 design is $\langle x_1^2 - x_1, x_2^2 - x_2, x_3^2 - x_3\rangle$. The origin is removed with the ideal operation $\mathrm{Ideal}(2^3 \setminus \{(0,0,0)\}) = \mathrm{Ideal}(2^3) + \langle \sigma_3 - \sigma_2 + \sigma_1 - 1\rangle$, where $\sigma_3 - \sigma_2 + \sigma_1 - 1 = x_1x_2x_3 - x_1x_2 - x_1x_3 - x_2x_3 + x_1 + x_2 + x_3 - 1$. Extend the polynomial ring with y_1, y_2, y_3 and create the following ideal: $\mathrm{Ideal}(2^3 \setminus \{(0,0,0)\}) + \langle y_1 l - x_1, y_2 l - x_2, y_3 l - x_3\rangle \subset \mathbb{R}[x_1, x_2, x_3, y_1, y_2, y_3]$, where $l = x_1 + x_2 + x_3$. Eliminate the variables x_1, x_2, x_3, for instance with the CoCoA macro `Elim`. This last step gives a set of generators for Ideal$(\mathcal{D})$ $\{y_1 + y_2 + y_3 - 1,\ y_3(y_3 - 1)(2y_3 - 1)(3y_3 - 1),\ y_2y_3(y_2 - y_3),\ y_3(2y_3 - 1)(2y_2 + y_3 - 1),\ y_2(2y_2 - 1)(y_2 + 2y_3 - 1)\}$.

In Scheffé (1963) Scheffé considers two types of fractions of a simplex centroid. A fraction $\mathcal{D}$ of the type in (Scheffé, 1963, §Appendix B) is built from a fraction of the 2^k design, $\mathcal{F}$ not including the origin. In this case Ideal$(\mathcal{D})$ is computed starting the above algorithm with $\mathcal{F}$ and by homogenization as in Theorem 2 Ideal$(\mathcal{C}_{\mathcal{D}})$ can be obtained. The ideal of a fraction of the other type (Scheffé, 1963, §5) is built starting the algorithm from an echelon fraction of the 2^k design excluding the origin. For echelon designs see (Pistone et al., 2001, §3.4). Some of the difficulties met by Scheffé (Scheffé, 1963, §Appendix B) in determining identifiably models for these fractions are then overcome by the algebraic approach to design, specifically the algorithms in Section 3.

Example 15 For $1 < m \leq k$ let $\mathcal{F}_m$ be the fraction of a simplex centroid design that includes all points with at most m non zero components, where $\mathcal{F}_k$ is the full simplex centroid. Clearly, $\mathcal{F}_m$ satisfies the description in (Scheffé, 1963, §5). The number of points in $\mathcal{F}_m$ is $\sum_{j=1}^{m}\binom{k}{j}$. The cone ideal for $\mathcal{F}_m$ is $\langle x_i^2 x_j - x_i x_j^2, x_{i_1}\cdots x_{i_{m+1}} : i \neq j \text{ and } i_1 \neq \cdots \neq i_{m+1}\rangle$ if $m > 1$ which for $m = 1$ simplifies to $\langle x_i x_j : i \neq j\rangle$. Differently from Example 12 the given generators are those of a saturated ideal.

Example 16 We compute the algebraic fan of $\mathcal{D} = \mathcal{F}_m$ of Example 15 as an example of the application of the techniques in Subsection 4.2. First note that the given generator set is a universal Gröbner basis. For $m = 1$ and any term ordering, the leading term of $x_i x_j \in \text{Ideal}(\mathcal{C}_\mathcal{D})$ is the monomial itself. Thus the homogeneous model has support $\{x_1^s, x_2^s, \ldots, x_k^s\}$ for any $s \in \mathbb{Z}_{\geq 1}$. If $m > 1$ the leading term of $x_{i_1}x_{i_2}\cdots x_{i_{m+1}}$ is the monomial itself. For a given initial term ordering on $x_1, \ldots, x_k$, e.g. $x_1 < x_2 < x_3$, the leading term of $x_i^2 x_j - x_i x_j^2$ is $x_i^2 x_j$ if $x_i > x_j$ and $x_i x_j^2$ otherwise. For a given initial term ordering there are $\sum_{j=1}^{m}\binom{k}{j}$ monomials of total degree s not divisible by $x_i^2 x_j$, with $x_i > x_j$ and $x_{i_1}x_{i_2}\cdots x_{i_{m+1}}$, namely for $m = 3$ $\{x_i^s, x_i^{s-1}x_j, x_i^{s-2}x_j x_l : i, j, l = 1, \ldots, k, i < j < l\}$.

4.3 Snee-Marquardt designs

In Snee and Marquardt (1976) simplex screening designs which are axial designs are presented and now they are known as Snee-Marquardt designs. The Snee-Marquardt design in k factors, $\mathcal{M}$, is formed by the points

k vertices	$(1, 0, \ldots, 0), \ldots, (0, \ldots, 0, 1)$
1 centroid	$(\frac{1}{k}, \ldots, \frac{1}{k})$
k interior points	$(\frac{k+1}{2k}, \frac{1}{2k}, \ldots, \frac{1}{2k}), \ldots, (\frac{1}{2k}, \ldots, \frac{1}{2k}, \frac{k+1}{2k})$
k end effects	$(0, \frac{1}{k-1}, \ldots, \frac{1}{k-1}), \ldots, (\frac{1}{k-1}, \ldots, \frac{1}{k-1}, 0)$

To construct Ideal($\mathcal{M}$) observe that each point in $\mathcal{M}$ lies on the line A_i through The ith vertex and its opposite end effect point, for $i = 1, \ldots, k$. The ideal Ideal($\mathcal{M} \cap \mathcal{A}_i$) is generated by $g = \sum_{i=1}^{k} x_i - 1$, $f_i = x_i x_l(x_i - (k+1)x_l)(x_i - x_l)$ where $l \in \{1, \ldots, i-1, i+1, \ldots, k\}$ and $x_j - x_l$, $1 \leq j < l \leq k$, $j \neq i$, $l \neq i$. The ideals of other types of axial designs are obtained by changing the f_i polynomials. First we prove that if h, l are different from i, then $x_i x_l (x_i - (k+1)x_l)(x_i - x_l)$ and $x_i x_h (x_i - (k+1)x_h)(x_i - x_h)$ cut A_i on the same subset. This remark justifies the fact that, in our notation, f_i does not depend on l. In fact, it holds $x_i x_l (x_i - (k+1)x_l)(x_i - x_l) - x_i x_h (x_i - (k+1)x_h)(x_i - x_h) = (x_l - x_h)x_i[x_i^2 - (k+2)x_i(x_l + x_h) + (k+1)(x_l^2 + x_l x_h + x_h^2)] \in \mathrm{Ideal}(A_i)$. The ideal defining $\mathcal{M}$ is the intersection of the $\mathrm{Ideal}(\mathcal{M} \cap \mathcal{A}_i)$'s. As usual we compute $\mathrm{Ideal}(\mathcal{C}_\mathcal{M})$. If $k = 3$, a straightforward computation shows that $\mathrm{Ideal}(\mathcal{C}_\mathcal{M}) = \langle (x_1 - x_2)(x_1 - x_3)(x_2 - x_3), x_1 x_2 (x_1 - x_2)(x_1 + x_2 - 5x_3), x_1 x_3 (x_1 - x_3)(x_1 + x_3 - 5x_2), x_2 x_3 (x_2 - x_3)(x_2 + x_3 - 5x_1) \rangle$. Next, we want to compute a finite generating set of $\mathrm{Ideal}(\mathcal{C}_\mathcal{M})$ for $k \geq 4$.

Proposition 1 *For $k \geq 4$, $\mathrm{Ideal}(\mathcal{C}_\mathcal{M})$ is generated by $q_{ijkl} = (x_i - x_j)(x_h - x_l)$ where i, j, h, l are different from each other in $\{1, \ldots, k\}$ and by $f_{rs} = x_r x_s (x_r - x_s)(x_r + x_s - (k+1)x_t))$, where r, s, t are different from each other in $\{1, \ldots, k\}$.*

A corollary of Proposition 1 is that

$$\mathrm{HF}_{\mathrm{Ideal}(\mathcal{C}_\mathcal{M})}(s) = \begin{cases} 1 & \text{if } s = 0 \\ k & \text{if } s = 1 \\ 2k & \text{if} s = 2 \\ 3k & \text{if} s = 3 \\ 3k+1 & \text{if} s \geq 4 \end{cases}$$

5 Notes on the analysis of two data sets

5.1 A non regular mixture design

In Giglio et al. (2001) a non-regular mixture experiment with $k = 8$ and $n = 18$ is analyzed. For the initial term ordering $h \prec g \prec f \prec e \prec d \prec c \prec b \prec a$ on the factors a hierarchical slack model for the response is obtained. For the same initial ordering the support for a homogeneous saturated model of degree 2 is $\{df, ef, f^2, ag, bg, cg, dg, eg, fg, g^2, ah, bh, ch, dh, eh, fh, gh, h^2\}$. Call it M_1. We could have chosen a submodel following the order ideal property. Some of the terms in M_1 are replaced by terms of different degree using the algorithm in Subsection 3.1.

Initial model	Final terms	R^2	R^2_A	$\hat{\sigma} \times 10^2$
M_1	h^2, bh, df, eh	0.977	0.958	6.1
M_2	f, h, bh, fh	0.983	0.978	4.4
M_3	$\frac{ef}{(1-e)(1-f)}, \frac{g^2}{(1-g)^2}, \frac{bh}{(1-b)(1-h)}, \frac{ch}{(1-c)(1-h)}, \frac{gh}{(1-g)(1-h)}$	0.974	0.964	5.7

Table 2: Results of model selection

In particular we may want to check if we can replace the quadratic terms of f^2, g^2, h^2 by the linear terms f, g, h. Indeed that is the case and we have a (more) Scheffé (like) model, named M_2. We could as well have replaced some interactions terms with linear terms, for example building models degree by degree using a suitable δ set in the algorithm in Subsection 3.1. But we do not pursue this here. Finally, following Cornell (2002) we can construct a support for a third model where $x_i x_j$ in M_1 are replaced by the rational terms $x_i x_j/((1-x_i)(1-x_j))$. We refer to this model as M_3. Such a substitution with rational terms is not always possible. But in this specific example it can be shown that the linear independence of the terms in M_3 over the design follows from the linear independence of the terms in M_1, because of the particular structure of the design.

For practical purposes, often a reduced model which fits reasonably well to the data, is preferred to the saturated one. Table 5.1 shows the values of the determination coefficient R^2, the adjusted one R^2_A and the residual error $\hat{\sigma}$ for the submodels obtained with backward stepwise regression. We use the `leaps` function in the statistical software `R`; see http://cran.r-project.org.

5.2 A fraction of the simplex centroid design

A particular fraction of the simplex centroid with k factors is proposed in McConkey et al. (2000) for screening for significant interactions. It exhibits some sort of symmetries. The fraction is constructed by considering the k corners of the simplex and those combinations with p non zero factors such that any pair of non zero factors appears in the design just once. The fact that there are many such fractions, obtained by relabeling of the factors is clearest from the structure of the polynomial representation below. The fraction obtained is of the echelon type described in (Scheffé, 1963, §5), and it is labeled $\{k|p\}$ in McConkey et al. (2000). In McConkey et al. (2000) it is noted that there are some values of k for which a $\{k|p\}$ fraction cannot be constructed. We focus our attention on the $\{9|3\}$ analysed in McConkey et al. (2000). To construct the cone ideal consider the polynomials

$$x_i(x_j - x_k), x_j(x_i - x_k), x_k(x_j - x_i) : (i, j, k) \in A \text{ and } x_i x_j(x_i - x_j) : i \neq j, i, j \in \{1, \ldots, 9\}$$

where the second set of polynomials gives the simplex centroid design in 9 factors and the set $A = \{(1,2,3), (1,4,8), (2,5,9), (3,6,7), (4,5,6), (2,4,7), (3,5,8), (1,6,9), (7,8,9), (1,5,7), (2,6,8), (3,4,9)\}$ corresponds to the non-zero triplets in our design. The centroid point $(1 : \ldots : 1)$ still satisfies that set of equations. The algebraic operation to remove it is the *colon* of ideals (Cox et al., 1997, Ch.4§4) and can be achieved by taking the saturation of the ideal generated by the above polynomials and $x_1x_2x_3x_4x_5x_6x_7x_8x_9$ or any other degree three monomial with exponents not in A, for example $x_4x_8x_9$, where the saturation is with respect to the usual ideal $\text{Ideal}(x_1, \ldots, x_9)$. The Hilbert function (Appendix 8.4) of the cone ideal is

$$\text{HF}_{\text{Ideal}(\mathcal{C}_\mathcal{D})}(s) = \begin{cases} 1 & \text{if } s = 0 \\ 9 & \text{if } s = 1 \\ 21 & \text{if } s \geq 2 \end{cases}$$

and thus we can construct a saturated homogeneous model of degree two. For the default term ordering in CoCoA with $x_1 > \ldots > x_9$ the support for such a model is

$$\begin{aligned} &\{x_1^2, x_2^2, x_2x_3, x_3^2, x_4^2, x_4x_7, x_4x_8, x_4x_9, x_5^2, x_5x_6, x_5x_7, x_5x_8, x_5x_9, x_6^2, \\ &x_6x_7, x_6x_8, x_6x_9, x_7^2, x_8^2, x_8x_9, x_9^2\} \end{aligned} \tag{7}$$

A feature of a $\{k|p\}$ fraction is that double interactions are completely confounded over the design in sets of size p, e.g. for the $\{9|3\}$ fraction the polynomials $x_1x_2 - x_1x_3, x_1x_2 - x_2x_3$ and $x_1x_3 - x_2x_3$ belong to $\text{Ideal}(\mathcal{C}_\mathcal{D})$, that is the column of a design/model involving the polynomials x_1x_2, x_2x_3 and x_1x_3 are equal. For this reason the analysis in (McConkey et al., 2000, Eqn.(3)) includes the sum $x_1x_2 + x_1x_3 + x_2x_3$.

The terms x_i can replace the terms x_i^2 in Equation (7), e.g. by application of the algorithm in Section 3.1. The design/model matrix for the obtained model and the fraction $\{9|3\}$ is a diagonal matrix of the form

$$\left[\begin{array}{c|c} I_9 & 0 \\ \hline P & \frac{1}{9}I_{12} \end{array}\right]$$

where I_k is the identity matrix of size k and P is the 12×9 matrix listing the coordinates of the mixture points.

6 Further comments

If the points of $\mathcal{D}$ do not lie on a hyperplane, none of them is the origin and each line through the origin and a design point does not contain any other design point, then the cone ideal is still well defined. The identifiability theory of homogeneous model supports works exactly as for mixture designs. In particular $\mathrm{Ideal}(\mathcal{C}_{\mathcal{D}})$ is the largest homogeneous ideal in $\mathrm{Ideal}(\mathcal{D})$. Although mathematically sensible, this operation does not seem to be reasonable if the design points do not lie on a hyperplane.

For an experiment where the relative proportions of the components are significant rather than the total amount, few relevant facts are implied by considering the cone ideal. The design points are recovered as the variety obtained from intersecting the cone ideal with the simplex ideal as shown in Theorem 1. The generalised confounding relationships collected in $\mathrm{Ideal}(\mathcal{C}_{\mathcal{D}})$ are the same whatever the total amount of the mixture is. Likewise the homogeneous model supports are independent of the total mixture amount.

Both the confounding relationships and the model support are easily computed even for fairly irregular designs, i.e. designs that do not manifest any geometric symmetry. An exact evaluation of the speed of the algorithms in function of the sample size and number of factors has not been done. An estimation can be obtained from Abbott et al. (2000). Macros in the computational algebra package CoCoA to compute homogeneous model supports, the ideals and the cone ideals of the designs in Section 4 are available from the first author.

A general remark on the algebraic statistics approach is that it allows a symbolic approach to identifiability. Thus numerical approximations are postponed to the estimation phase of an analysis. For example rather than checking numerically if the rank of the design/model matrix for a candidate model is maximal, one computes a basis of the quotient space. This might be advantageous or disadvantageous according to the practical situations. We find that the information embedded in the ideal of a design or of its cone are useful in visualising the constraints imposed on the power terms by the design.

7 Acknowledgments

The authors thank Prof. H. P. Wynn and A. di Bucchianico for providing initial bibliographical references on mixture designs. The first author acknowledges financial support from CONACYT.

8 Appendix

Reference texts for this appendix include Adams and Loustaunau (1994); Cox et al. (1997); Kreuzer and Robbiano (2000).

8.1 Basic concepts

With $\mathbb{R}[x_1, \ldots, x_k]$ we indicate the set of polynomials in $x_1, \ldots, x_k$ and with real coefficients. The theory holds for whatever field K instead of $\mathbb{R}$. For us T^k indicates the set of power products or monomials in $\mathbb{R}[x_1, \ldots, x_k]$: $x^\alpha = x_1^{\alpha_1} \ldots x_k^{\alpha_k}$ for $\alpha_i \in \mathbb{Z}_{\geq 0}$ and a polynomial $f \in \mathbb{R}[x_1, \ldots, x_k]$ is a finite sum $f = \sum_{\alpha \in A} a_\alpha x^\alpha$ with $x^\alpha \in T^k$, $a_\alpha \in \mathbb{R}$ and for a finite subset $A \subset \mathbb{Z}^k_{\geq 0}$.

Definition 3 *A set $I \subset \mathbb{R}[x_1, \ldots, x_k]$ is a polynomial ideal if i) $f + g \in I$ for all $f, g \in I$ and ii) $hf \in I$ for all $h \in \mathbb{R}[x_1, \ldots, x_k]$ and $f \in I$.*

We state the very deep property of polynomial ideals known as the Hilbert Basis Theorem (Cox et al., 1997, Ch.2§5)

Theorem 9 *Every ideal $I \subseteq \mathbb{R}[x_1, \dots, x_k]$ is finitely generated, i.e. there exist $g_1, \dots, g_t \in I$ such that for every $f \in I$ there exist $h_1, \dots, h_t \in \mathbb{R}[x_1, \dots, x_k]$ that satisfy $f = h_1 g_1 + \cdots + h_t g_t$.*

The polynomials $g_1, \dots, g_t$ in the previous theorem form a set of generators of I and we write $I = \langle g_1, \dots, g_t \rangle$. There are special sets of generators called Gröbner bases. To introduce them we need the notion of term ordering. A term ordering τ is a total order relation on T^k that satisfies *i)* $x^\alpha > 1$ for all non zero $\alpha \in \mathbb{Z}^k_{\geq 0}$ and *ii)* if $x^\alpha > x^\beta$ then $x^\alpha x^\gamma > x^\beta x^\gamma$ for all $\alpha, \beta, \gamma \in \mathbb{Z}^k_{\geq 0}$.

Definition 4 *Given a term ordering τ, the leading term of a polynomial $f \in \mathbb{R}[x_1, \dots, x_k]$ is its largest term with respect to τ, and we write it as $\mathrm{LT}_\tau(f)$.*

Given a term ordering τ and an ideal I, we consider the set of leading terms of all polynomials in I: $\mathrm{LT}_\tau(I) = \langle \mathrm{LT}_\tau(f) : f \in I \rangle$. If $g_1, \dots, g_t$ is a generator set of an ideal I, in general $\mathrm{LT}_\tau(g_1)$, $\dots$,, $\mathrm{LT}_\tau(g_t)$ is not a set of generators of $\mathrm{LT}_\tau(I)$. This remark justifies the following definition.

Definition 5 *Let I be an ideal, τ a term ordering and $G = \{g_1, \dots, g_t\} \subseteq I$. G is a Gröbner basis (sometimes called a standard basis) of I if $\mathrm{LT}_\tau(I)$ is generated by $\langle \mathrm{LT}_\tau(g) : g \in G \rangle$.*

Theorem 10 *For every ideal I and term ordering τ there exist Gröbner bases of I.*

Definition 6 *Let $r = \sum_{\alpha \in A} a_\alpha x^\alpha$ be a polynomial, τ a term ordering and I be an ideal. r is in normal form w.r.t. I and τ if $x^\alpha \notin \mathrm{LT}_\tau(I)$ for all $\alpha\ inA$.*

The following result holds.

Proposition 2 *Let τ be a term ordering, I an ideal and let $G = \{g_1, \dots, g_t\}$ be a Gröbner basis of I w.r.t. τ. For every polynomial $f \in \mathbb{R}[x_1, \dots, x_k]$ there exists a unique $r \in \mathbb{R}[x_1, \dots, x_k]$ in normal form and $h_1, \dots, h_t \in \mathbb{R}[x_1, \dots, x_k]$ such that $f = h_1 g_1 + \cdots + h_t g_t + r$. Furthermore, $r = 0$ if and only if $f \in I$.*

Given an ideal I, we can consider the quotient ring $\mathbb{R}[x_1, \dots, x_k]/I$ whose elements are the equivalence classes $[f]$ of the relation $f \sim g$ if $f - g \in I$. It is easy to prove that if r is the normal form of f w.r.t. I and τ, then $[f] = [r]$ and so the elements of $\mathbb{R}[x_1, \dots, x_k]/I$ (are represented) by polynomials obtained as combination of terms not in $\mathrm{LT}_\tau(I)$. The set $\mathrm{SM}_\tau(I) = T^k \setminus \mathrm{LT}_\tau(I)$ is called the set of the standard monomials of I w.r.t. τ. As $\mathbb{R}$-vector spaces, $\mathbb{R}[x_1, \ldots, x_k]/I$ is isomorphic to $\mathbb{R}[x_1, \ldots, x_k]/\mathrm{LT}_\tau(I)$ and so it is isomorphic to the vector space spanned by $\mathrm{SM}_\tau(I)$ over $\mathbb{R}$. The Singular macro *kbasis* returns $\mathrm{SM}_\tau(I)$ for an ideal of points.

8.2 Affine Hilbert function for ideals

For $s \in \mathbb{Z}_{\geq 0}$ let $\mathbb{R}[x_1, \ldots, x_k]_{\leq s} = \mathrm{Span}(x^\alpha \in T^k : \sum_{i=1}^k \alpha_i \leq s)$. For an ideal $I \subset \mathbb{R}[x_1, \ldots, x_k]$, let $I_{\leq s} = I \cap \mathbb{R}[x_1, \ldots, x_k]_{\leq s}$. As $\mathbb{R}[x_1, \ldots, x_k]_{\leq s}$ is a $\mathbb{R}$-vector space of dimension $\binom{k+s}{s}$ and $I_{\leq s}$ is a subvector space of $\mathbb{R}[x_1, \ldots, x_k]_{\leq s}$, we can define the *affine Hilbert function* of I as

$$^{\mathrm{a}}\mathrm{HF}_I(s) = \dim \mathbb{R}[x_1, \ldots, x_k]_{\leq s}/I_{\leq s} = \dim \mathbb{R}[x_1, \ldots, x_k]_{\leq s} - \dim I_{\leq s}.$$

There exists s_0 called the *index of regularity of* I such that for all $s \geq s_0$ $^{\mathrm{a}}\mathrm{HF}_I(s)$ is a polynomial with integer coefficients. It is called the *affine Hilbert polynomial* of I and denoted as $^{\mathrm{a}}\mathrm{HP}_I(s)$. That is

$$^{\mathrm{a}}\mathrm{HP}_I(s) = \sum_{i=0}^{k} b_i \begin{pmatrix} s \\ k-i \end{pmatrix}$$

with $b_i \in \mathbb{Z}_{\geq 0}$ and $b_i > 0$. The following theorem gives the affine Hilbert function for the design ideal $I(\mathcal{D})$.

Theorem 11 *Let $I(\mathcal{D})$ be the ideal generated by a design $\mathcal{D}$ with n distinct points. Then for $s \geq n$, $^{\mathrm{a}}\mathrm{HF}_{I(\mathcal{D})}(s) = {}^{\mathrm{a}}\mathrm{HP}_{I(\mathcal{D})}(s) = n$.*

Proof. This is in (Cox et al., 1997, Ex.10,Ch.9§4). ∎

The Hilbert function counts the monomials that are not in $I(\mathcal{D})$; this set of monomials is precisely the set of standard monomials as described in Subsection 8.1. As $^{\mathrm{a}}\mathrm{HP}_{I(\mathcal{D})}(s)$ is a constant, we retrieve the standard result $\dim \mathbb{R}[x_1, \ldots, x_k]/I = n$.

A term ordering τ is graded if x^α is larger than x^β whenever $\sum_{i=1}^k \alpha_i > \sum_{i=1}^k \beta_i$. Let τ be a graded term ordering, then for all $s \in \mathbb{Z}_{\geq 0}$

$$^{\mathrm{a}}\mathrm{HF}_I(s) = \#\left(\mathrm{SM}_\tau(I) \cap \mathbb{R}[x_1, \ldots, x_k]_{\leq s}\right)$$

where $\#A$ is the size of the set A.

8.3 Homogenising a mixture ideal

A key point in this paper is the study of mixture designs through cone ideals, namely $\mathrm{Ideal}(\mathcal{C}_{\mathcal{D}}) \subset \mathbb{R}[x_1, \ldots, x_k]$ for a mixture design $\mathcal{D}$. As mentioned in the main text, there are macros e.g. `IdealOfProjectivePoints` which construct a generator set for $\mathrm{Ideal}(\mathcal{C}_{\mathcal{D}})$ from the coordinates of $\mathcal{D}$. Next we outline the basic construction of $\mathrm{Ideal}(\mathcal{C}_{\mathcal{D}})$ which can be performed in any software for ideal computation. Let $\mathcal{D} = \{P_1, \ldots, P_n\}$ be the design and assume that $P_i = (a_{i1}, \ldots, a_{ik})$ with $\sum_{j=1}^{k} a_{ij} = 1$. Then, P_i belongs to the hyperplane H defined by the single equation $x_1 + \ldots + x_k = 1$ for $i = 1, \ldots, n$. Moreover P_i is the intersection of H with the line L_i containing P_i and the origin $0 = (0, \ldots, 0)$. In particular, we have $\mathrm{Ideal}(\{P_i\}) = \langle \mathrm{Ideal}(\{L_i\}), x_1 + \ldots + x_k - 1\rangle$. But $\mathrm{Ideal}(\mathcal{D}) = \bigcap_{i=1}^{n} \mathrm{Ideal}(\{P_i\}) = \langle \bigcap_{i=1}^{n} \mathrm{Ideal}(\{L_i\}), x_1 + \ldots + x_k - 1\rangle$. We set $\mathrm{Ideal}(\mathcal{C}_{\mathcal{D}}) = \bigcap_{i=1}^{n} \mathrm{Ideal}(\{L_i\})$, and so $\mathrm{Ideal}(\mathcal{D}) = \langle \mathrm{Ideal}(\mathcal{C}_{\mathcal{D}}), x_1 + \ldots + x_k - 1\rangle$. Now, we describe some properties of $\mathrm{Ideal}(\mathcal{C}_{\mathcal{D}})$.

Theorem 12 $\mathrm{Ideal}(\mathcal{C}_{\mathcal{D}})$ *is generated by homogeneous polynomials.*

Proof. The ideal defining the lines L_i is generated by the 2×2 minors of the matrix

$$\begin{pmatrix} x_1 & \ldots & x_k \\ a_{i1} & \ldots & a_{ik} \end{pmatrix}$$

and so it is generated by homogeneous linear polynomials. The intersection of ideals generated by homogeneous polynomials is again generated by homogeneous polynomials. So the claim follows. ∎

$\mathrm{Ideal}(\mathcal{C}_{\mathcal{D}})$ can be characterized as follows.

Theorem 13 $\mathrm{Ideal}(\mathcal{C}_{\mathcal{D}})$ *is the largest homogeneous ideal in* $\mathrm{Ideal}(\mathcal{D})$.

Proof. Let $f \in \mathrm{Ideal}(\mathcal{D})$, f homogeneous. Then $f(ta_{i1}, \ldots, ts_{ik}) = t^{\deg f} f(a_{i1}, \ldots, f_{ik}) = 0$ for every $i = 1, \ldots, n$ and for all $t \in \mathbb{R}$. Hence, $f \in \mathrm{Ideal}(\{L_i\})$ for all $i = 1, \ldots, n$ and so $f \in \mathrm{Ideal}(\mathcal{C}_{\mathcal{D}})$. That is every homogeneous polynomial in $\mathrm{Ideal}(\mathcal{D})$ is in $\mathrm{Ideal}(\mathcal{C}_{\mathcal{D}})$ and the claim follows. ∎

8.4 Hilbert function

An ideal $I^h \subset \mathbb{R}[x_1,\ldots,x_k]$ is homogeneous if it is generated by a set of homogeneous polynomials. For $s \in \mathbb{Z}_{\geq 0}$ let $\mathbb{R}[x_1,\ldots,x_k]_s = \mathrm{Span}(x^\alpha \in T^k : \sum_{i=1}^k \alpha_i = s) \cup \{0\}$ and for a homogeneous ideal $I^h \subset \mathbb{R}[x_1,\ldots,x_k]$, let $I^h_s = I^h \cap \mathbb{R}[x_1,\ldots,x_k]_s$. $\mathbb{R}[x_1,\ldots,x_k]_s$ is a $\mathbb{R}$-vector space of dimension $\binom{k+s-1}{s}$ and I^h_s is a subvector space. The Hilbert function of the homogeneous ideal I is $\mathrm{HF}_I(s) = \dim \mathbb{R}[x_1,\ldots,x_k]_s / I^h_s$.

Theorem 14 *Let $I^h \subset \mathbb{R}[x_1,\ldots,x_k]$ be a homogeneous ideal.*

1. *For s sufficiently large $\mathrm{HF}_{I^h}(s)$ is a polynomial with rational coefficients and integer values.*
2. *For $s \geq 1$*
$$\mathrm{HF}_{I^h}(s) = {}^{\mathrm{a}}\mathrm{HF}_{I^h}(s) - {}^{\mathrm{a}}\mathrm{HF}_{I^h}(s-1) \tag{8}$$
3. *If I^h is a monomial ideal and thus trivially homogeneous, then $\mathrm{HF}_{I^h}(s)$ is the number of monomials not in I^h and in $\mathbb{R}[x_1,\ldots,x_k]_s$.*
4. *If τ is a term ordering and I^h a homogeneous ideal, then $\mathrm{HF}_{I^h}(s) = \mathrm{HF}_{\langle \mathrm{LT}(I^h)\rangle}(s)$.*
5. `(The dimension theorem)` *Let $V = V(I) = \left\{a \in \mathbb{P}^{k-1}(\mathbb{C}) : f(a) = 0 \text{ for all } f \in I\right\}$ be non empty. Then $\dim(V) = \deg \mathrm{HP}_I(s)$ where $\dim(V)$, for V a projective variety, is defined as the degree of the Hilbert polynomial of I. Furthermore, $\dim(V) = \deg \mathrm{HP}_{\langle \mathrm{LT}(I)\rangle}(s)$ equals the maximum dimension of a projective coordinate subspace in $V(\langle \mathrm{LT}(I)\rangle)$. If $I = \mathrm{Ideal}(V)$ the last statements hold over $\mathbb{R}$.*
6. *The previous statement holds for I an ideal, not necessarily homogeneous, $V = V(I)$ and $\mathrm{HP}_I(s)$ is substituted by ${}^{\mathrm{a}}\mathrm{HP}_I(s)$*

For the proof we refer to any classical text such as Cox et al. (1997). Here we just need to observe that as we deal with a regular structure as $V = \mathcal{C}_\mathcal{D}$ then $I = \mathrm{Ideal}(V)$.

The CoCoA macro `Hilbert` applied to a homogeneous ideal computes the Hilbert function of the ideal. In Singular we use `hilb` and `vdim`. The affine Hilbert function of the homogeneous

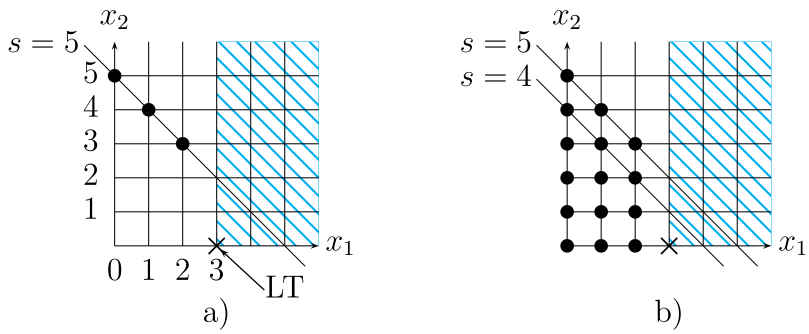

Figure 2: Standard monomials counted by a) the Hilbert function with $s = 5$ and b) the affine Hilbert function for $s = 4, 5$. Both cases refer to $\mathrm{I}(\mathcal{C}_\mathcal{D})$ of Example 17.

ideal can be retrieved by Equation (8) together with the initial condition ${}^{\mathrm{a}}\mathrm{HF}_{I^h}(0) = 1$. If the ideal is not homogeneous then `Hilbert` returns the Hilbert function of the corresponding leading term ideal w.r.t. whatever term ordering is running in the open computer session.

Example 17 For $\mathcal{D} = \{(1/2, 1/2), (1/4, 3/4), (0, 1)\}$ and a term order in which $x_1 > x_2$, $\mathrm{Ideal}(\mathcal{C}_\mathcal{D}) = \langle x_1^3 - 4/3x_1^2x_2 + 1/3x_1x_2^2\rangle$. Compare the following table with Figure 2

s	$\mathrm{HF}_{\mathrm{Ideal}(\mathcal{C}_\mathcal{D})}(s)$	${}^a\,\mathrm{HF}_{\mathrm{Ideal}(\mathcal{C}_\mathcal{D})}(s)$
0	1	1
1	2	3
2	3	6
3	3	9
4	3	12
$\vdots$	3	$3 + {}^a\,\mathrm{HF}_{\mathrm{Ideal}(\mathcal{C}_\mathcal{D})}(s-1)$

Theorem 15 *Let $\mathcal{D}$ be a mixture design with n distinct points and let $\mathcal{C}_\mathcal{D}$ be its cone; let* $\mathrm{Ideal}(\mathcal{D})$ *and* $\mathrm{Ideal}(\mathcal{C}_\mathcal{D})$ *be their corresponding ideals. Then for s large enough,* $\mathrm{HF}_{I(\mathcal{C}_\mathcal{D})}(s) = {}^{\mathrm{a}}\mathrm{HF}_{I(\mathcal{D})}(s)$.

Proof. This is Theorem 4. ■

Example 18 The Hilbert function of the cone ideal of the $\{4, 4\}$ design in Example 12 is

$$\mathrm{HF}_{\mathrm{Ideal}(\mathcal{C}_{\mathcal{D}})}(s) = \begin{cases} 1 & \text{if } s = 0 \\ 4 & \text{if } s = 1 \\ 10 & \text{if } s = 2 \\ 20 & \text{if } s = 3 \\ 35 & \text{if } s \geq 4 \end{cases}$$

For the fraction cut by $(x_1 - x_2)(x_3 - x_4)$ it is

$$\mathrm{HF}_{\mathrm{Ideal}(\mathcal{C}_{\mathcal{F}})}(s) = \begin{cases} 1 & \text{if } s = 0 \\ 4 & \text{if } s = 1 \\ 9 & \text{if } s = 2 \\ 13 & \text{if } s = 3 \\ 15 & \text{if } s \geq 4 \end{cases}$$

We use the CoCoA macro `Hilbert`.

8.5 Proofs

Proof. of Theorem 1. *1.* Let $f \in I = \{f \in \mathbb{R}[x_1, \ldots, x_k] : f$ is homogeneous and $f(d) = 0$ for all $d \in \mathcal{D}\}$. As f is homogeneous then $f(\alpha d) = 0$ for all $\alpha \in \mathbb{R}$ and thus $f(d) = 0$ for $d \in \mathcal{C}_{\mathcal{D}}$. Hence $I \subseteq \mathrm{Ideal}(\mathcal{C}_{\mathcal{D}})$.

Now we show that $\mathrm{Ideal}(\mathcal{C}_{\mathcal{D}})$ is homogeneous. If $f \in \mathbb{R}[x_1, \ldots, x_k]$ and $f(d) = 0$ on the cone then as $\mathcal{D} \subset \mathcal{C}_{\mathcal{D}}$ $f(d) = 0$ on $\mathcal{D}$. Any polynomial f can be written as $f = f_s + f_{s-1} + \cdots + f_0$ with f_i homogeneous polynomials of degree i. For $\alpha \in \mathbb{R}$ and $d \in \mathbb{R}^k$

$$f(\alpha d) = f_s(\alpha d) + f_{s-1}(\alpha d) + \cdots + f_0(\alpha d) = \alpha^s f_s(d) + \alpha^{s-1} f_{s-1}(d) + \cdots + \alpha^0 f_0(d) \qquad (9)$$

If we take f vanishing on $\mathcal{C}_{\mathcal{D}}$ then we have $f(\alpha d) = 0$ for all $\alpha \in \mathbb{R}$ and $d \in \mathcal{D}$. Equation (9) is a polynomial of degree s in α. As it is zero for infinitely many α's then its coefficients are zero that is $f_s(d) = \ldots = f_0(d) = 0$. In particular for all $d \in \mathcal{D}$. As by construction f_i is homogeneous, $f_j(d) = 0$ for all d in the cone. Hence $\mathrm{Ideal}(\mathcal{C}_{\mathcal{D}}) + \langle \sum_{i=1}^k -1 \rangle \subseteq \mathrm{Ideal}(\mathcal{D})$.

2. Clearly $\text{Ideal}(\mathcal{C}_D) \subsetneq \text{Ideal}(\mathcal{D}) \subset \mathbb{R}[x_1, \ldots, x_k]$ and $\langle \sum_{i=1}^k x_i - 1\rangle \subsetneq \text{Ideal}(\mathcal{D}) \subset \mathbb{R}[x_1, \ldots, x_k]$. Hence, $\text{Ideal}(\mathcal{C}_D) + \langle \sum_{i=1}^k x_i - 1\rangle \subseteq \text{Ideal}(\mathcal{D})$.

Let $g \in \text{Ideal}(\mathcal{D})$. Then there exists $s \in \mathbb{Z}_{\geq 0}$ such that $g = \sum_{i=0}^s f_i$ and the f_i's are homogeneous polynomials of total degree i. As $\sum_{i=1}^k x_i - 1 \in \text{Ideal}(\mathcal{D})$ we set $\sum_{i=0}^s f_i(x_1 + \cdots + x_k)^{s-i} = h(g)$ over $\mathcal{D}$. Then, for $l = x_1 + \cdots + x_k$

$$\begin{aligned} g - h(g) &= g - \textstyle\sum_{i=0}^s f_i(x_1 + \cdots + x_k)^{s-i} = g - \sum_{i=0}^s f_i l^{s-i} \\ &= (1-l)\left(f_{s-1} + (1+l)f_{s-2} + \cdots + (1 + l + \cdots + l^{s-1})f_0\right) = (1-l)\bar{f} \end{aligned}$$

and we have $g - h(g) = \bar{f}(1-l)$. But both g and $(1-l)\bar{f}$ are in $\text{Ideal}(\mathcal{D})$, thus $h(g) \in \text{Ideal}(\mathcal{D})$. By 1. $h(g) \in \text{Ideal}(\mathcal{C}_\mathcal{D})$ and thus $g \in \text{Ideal}(\mathcal{C}_\mathcal{D}) + \langle l - 1\rangle$ and the the proof is concluded. ∎

Proof. of Theorem 2. Let $f \in \text{Ideal}(\mathcal{D})$ be a homogeneous polynomial of degree s. From the defining property of a Gröbner basis, there exist $q, q_1, \ldots, q_r \in \mathbb{R}[x_1, \ldots, x_k]$ such that $f = q(l-1) + q_1 g_1 + \ldots + q_r g_r$ with $\deg q \leq s - 1$ and $\delta_i = \deg(q_i g_i) \leq s$. Homogenising we obtain $h(f) = h(q)h(l-1) + l^{s-\delta_1}h(q_1)h(g_1) + \ldots + l^{s-\delta_r}h(q_r)h(g_r)$ and of course $h(l-1) = l - l = 0$. Thus $h(f) = \sum_{i=1}^r l^{s-\delta_i}h(q_i)h(g_i)$. But f is homogeneous and so $f = h(f)$ and $f = \sum_{i=1}^r l^{s-\delta_i}h(q_i)h(g_i)$. The claim now follows from Theorem 1. ∎

Proof. of Lemma 3. Let $[f]$ be an element in $\mathbb{R}[x_1, \ldots, x_k]_{\leq s}/\,\text{Ideal}(\mathcal{D})_{\leq s}$. We want to prove that there exists $g \in [f]$ such that g is homogeneous of degree s. Let $l = x_1 + \ldots + x_k$ and let $f = f_t + \ldots + f_0$ where f_j is homogeneous of degree j and $t \leq s$. Let $g = l^{s-t}\left(f_t + lf_{t-1} + \ldots + l^t f_0\right) l^{s-t}h(f)$. Then,

$$\begin{aligned} g - f &= l^{s-t}\left(f_t + lf_{t-1} + \ldots + l^t f_0\right) - \left(f_t + lf_{t-1} + \ldots + l^t f_0\right) \\ &\quad + \left(f_t + lf_{t-1} + \ldots + l^t f_0\right) - (f_t + \ldots + f_0) \\ &= (l^{s-t} - 1)\left(f_t + lf_{t-1} + \ldots + l^t f_0\right) + (l-1)f_{t-1} + (l^2 - 1)f_{t-2} + \ldots + (l^t - 1)f_0 \\ &= (l-1)\left[(l^{s-t-1} + \ldots + 1)\left(f_t + lf_{t-1} + \ldots + l^t f_0\right)\right. \\ &\quad \left. + f_{t-1} + (l+1)f_{t-2} + \ldots + (l^{t-1} + \ldots + 1)f_0\right] \end{aligned}$$

But $l - 1 \in \text{Ideal}(\mathcal{D})$ and so $g \in [f]$. ∎

Proof. of Theorem 4. Let $[f_1], \ldots, [f_p]$ be a basis of the $\mathbb{R}$-vector space $\mathbb{R}[x_1, \ldots, x_k]_{\leq s}/\text{Ideal}(\mathcal{D})_{\leq s}$ and let $g_1, \ldots, g_p$ be the degree s homogeneous polynomials constructed in Lemma 3. We want to prove that $[g_1], \ldots, [g_p]$ is a basis of $\mathbb{R}[x_1, \ldots, x_k]_s/\text{Ideal}(\mathcal{C}_\mathcal{D})_s$. They are linearly independent:

assume there exist $\lambda_1, \ldots, \lambda_p \in \mathbb{R}$ such that $\lambda_1[g_1] + \ldots + \lambda_p[g_p] = 0$. Then $\lambda_1 g_1 + \ldots + \lambda_p g_p \in \text{Ideal}(\mathcal{C}_\mathcal{D}) \subseteq \text{Ideal}(\mathcal{D})$ and so $\lambda_1[g_1] + \ldots + \lambda_p[g_p] = 0$ in $\mathbb{R}[x_1, \ldots, x_k]_{\leq s}/\text{Ideal}(\mathcal{D})_{\leq s}$. Hence, $\lambda_1[f_1] + \ldots + \lambda_p[f_p] = 0$ and so $\lambda_1 = \ldots = \lambda_p = 0$ because $[f_1], \ldots, [f_p]$ is a basis of $\mathbb{R}[x_1, \ldots, x_k]_{\leq s}/\text{Ideal}(\mathcal{D})_{\leq s}$.

Let $g \in \mathbb{R}[x_1, \ldots, x_k]_s$. Thus, there exist $\lambda_1, \ldots, \lambda_p \in \mathbb{R}$ such that $[g] = \lambda_1[f_1] + \ldots + \lambda_p[f_p] = \lambda_1[g_1] + \ldots + \lambda_p[g_p]$ and so $[g_1], \ldots, [g_p]$ are generators of $\mathbb{R}[x_1, \ldots, x_k]_s/\text{Ideal}(\mathcal{C}_\mathcal{D})_s$. As a consequence, we get the claim. If s is sufficiently large then $\dim \mathbb{R}[x_1, \ldots, x_k]_{\leq s}/\text{Ideal}(\mathcal{D})_{\leq s} = n$ (see e.g. Pistone and Wynn (1996)) and thus $p = n$. ∎

Proof. of Theorem 5. It is easy to show that $\text{Ideal}(\mathcal{C}_\mathcal{D})$ is generated by $\langle x_i x_j : 1 \leq i, j \leq k, i \neq j \rangle$ and so $\text{Ideal}(\mathcal{D}) = \langle x_1 + \ldots + x_k - 1, x_i x_j : 1 \leq i, j \leq k, i \neq j \rangle$. A Gröbner basis of $\text{Ideal}(\mathcal{D})$ contains also the polynomials $x_i^2 - x_i$, obtained from the S-polynomial test (Cox et al., 1997, Ch.2§6Th.6) as $x_i(x_1 + \ldots + x_k - 1) - \sum_{i \neq j} x_i x_j$. The result now follows easily. ∎

Proof. of Theorem 6. For 1. observe that as the term ordering is graded then lower order terms are favoured over higher order terms and then included in the support for a slack model. It follows directly from the structure of the design/model matrix involved

$$
\begin{array}{c|cccc|c}
 & x_1 & \ldots & x_{k-1} & 1 & \cdots \\
\hline
(1,0,\ldots,0) & 1 & 0\ldots & 0 & 1 & \cdots \\
\vdots & & & & & 0 \\
(0,\ldots,1,0) & 0 & 0\ldots & 1 & 1 & \cdots \\
(0,\ldots,0,1) & 0 & 0\ldots & 0 & 1 & \cdots \\
\hline
\vdots & & & & &
\end{array}
$$

For 2. let $\text{NF}(x_k^{\alpha_k}) = \sum_{x^\alpha} \theta_\alpha x^\alpha$ where for a slack support no x^α involves x_k and evaluate it at the corner point $c_k = (0, \ldots, 0, 1)$. Deduce $\theta_0 = 1$. Similarly 3. is proved. ∎

Lemma 16 *Let $\mathcal{D}$ be a $\{k, m\}$ simplex lattice design. Then a basis of the $\mathbb{R}$-vector space $\mathbb{R}[x_1, \ldots, x_k]_{\leq s}/\ \text{Ideal}(\mathcal{D})_{\leq s}$ is $\{1, x_2, \ldots, x_k, x_2^2, x_2 x_3, \ldots, x_k^2, \ldots, x_2^{s'}, x_2^{s'} x_3, \ldots, x_k^{s'}\}$ where $s' = \min\{s, m\}$.*

Proof. The claim is equivalent to the following: $\text{Ideal}(\mathcal{C}_\mathcal{D})_s = 0$ for $s \leq m$. Indeed, $x_1 + \ldots + x_k - 1 \in \text{Ideal}(\mathcal{D})$ and we can choose the other generators of $\text{Ideal}(\mathcal{D})$ as homogeneous polynomials in Ideal($\mathcal{C}_{\mathcal{D}}$) by Theorem 1. Thus, let $f \in \text{Ideal}(\mathcal{C}_{\mathcal{D}})_m$. We want to prove that $f = 0$ and we use induction on k and m. The base of the induction is as follows. First, we analyse the case $\{2, m\}$, for which $\mathcal{D} = \{P_0, \ldots, P_m\}$ with $P_i = (i/m, (m-i)/m)$ for $i = 0, \ldots, m$. But no homogeneous polynomial of degree m can have $m+1$ distinct zeros, unless it is the null polynomial. Second, we consider the case $\{k, 1\}$. But this design was studied in Lemma 5.

Now, we consider the general case $\{k, m\}$ and we assume that no polynomial of degree $m-1$ belongs to a $\{k, m-1\}$ design and that no polynomial of degree m belongs to a $\{k-1, m\}$ design. Let $f \in \text{Ideal}(\mathcal{C}_{\mathcal{D}})_m$. We need to show that $f = 0$. If we set $x_k = 0$ then we obtain a $\{k-1, m\}$ design $\mathcal{D}'$ and $f(x_1, \ldots, x_{k-1}, 0) \in \text{Ideal}(\mathcal{C}'_{\mathcal{D}})_m$. By inductive hypothesis, $f(x_1, \ldots, x_{k-1}, 0)$ is the zero polynomial. Hence, $f = x_k f'$ for some f' suitable homogeneous polynomial f' of degree $m-1$. The affine transformation, $X_i = \frac{m}{m-1} x_i$, $i = 1, \ldots, k-1$ and $X_k = -\frac{1}{m-1} + \frac{m}{m-1} x_k$, takes $\mathcal{D} \setminus \mathcal{D}'$ into a $\{k, m-1\}$ simplex lattice design, say $\mathcal{D}''$, and f' into $\left(\frac{m}{m-1}\right)^{m-1} f'(X_1, \ldots, X_{k-1})$ $\in \text{Ideal}(\mathcal{D}'')$. By inductive hypothesis, we have $f' = 0$ and so $f = 0$. As a consequence the Hilbert function of $\mathcal{D}$ is

$$\dim \mathbb{R}[x_1, \ldots, x_k]_{\leq s} / \text{Ideal}(\mathcal{D})_{\leq 0} = 1 + \binom{k-1}{k-2} + \ldots + \binom{s'+k-2}{k-2} = \binom{s'+k-1}{k-1}$$

where $s' = \min\{s, m\}$ and the claim follows because $\binom{m+k-1}{k-1}$ is the number of points in $\mathcal{D}$. ∎

Proof. of Theorem 7. In order to respect the order ideal property, not all factors can be included in the presence of the intercept. Moreover no higher degree power in any factor can be included as shown in Lemma 16. ∎

Proof. of Corollary 8. Any other candidate model support would include the terms $1, x_1, , \ldots, x_k$, but they all cannot be identified as $x_1 + \ldots + x_k = 1$ over $\mathcal{D}$. ∎

Proof. of Proposition 1. Let J be the ideal generated by the q_{ijkl} and f_{rs}. First, we prove that if u, v are different from r, s then $x_r x_s (x_r - x_s)(x_r + x_s - (k+1)x_u))$ and $x_r x_s (x_r - x_s)(x_r + x_s - (k+1)x_v)$ are equivalent modulo the q_{ijkl}'s. In fact

$$x_r x_s (x_r - x_s)(x_r + x_s - (k+1)x_u)) - x_r x_s (x_r - x_s)(x_r + x_s - (k+1)x_v) = (k+2) x_r x_s (x_r - x_s)(x_u - x_v)$$

and the equivalence follows. Second, we know that $\text{Ideal}(\mathcal{C}_{\mathcal{M}}) = \cap_{i=1}^{k} \text{Ideal}(\mathcal{C}_{\mathcal{M} \cap A_i})$. Hence, if we prove that $J \subseteq \text{Ideal}(\mathcal{CM} \cap A_i)$, $i = 1, \ldots, k$, then we obtain that $J \subseteq \text{Ideal}(\mathcal{C}_{\mathcal{M}})$. Without loss of generality fix $i = 1$. Thus we have to prove that $J \subseteq \langle x_j - x_l, f_i : j, l \in \{1, \dots, k\}\rangle$. If we choose four different elements i, j, k, l in $\{1, \dots, k\}$, at least one between $x_i - x_j$ and $x_h - x_l$ belongs to $\text{Ideal}(\mathcal{C}_{\mathcal{M}\cap A_i})$, and so $q_{ijkl} \in \text{Ideal}(\mathcal{C}_{\mathcal{M}\cap A_1})$. If $r \neq 1$, $s \neq q$ the same argument shows that $f_{rs} \in \text{Ideal}(\mathcal{C}_{\mathcal{M}\cap A_1})$. But

$$\begin{aligned} f_{1s} - f_s &= x_1x_s(x_1 - x_s)(x_1 + x_s - (k+2)x_t) - x_1x_s(x_1 - (k+1)x_s)(x_1 - x_s) \\ &= (k+2)x_1x_s(x_1 - x_s)(x_s - x_t) \in \text{Ideal}(\mathcal{C}_{\mathcal{M}\cap\mathcal{A}_\infty}) \end{aligned}$$

because $s \neq 1$ and $t \neq 1, s$. Hence $J \subseteq \text{Ideal}(\mathcal{C}_{\mathcal{M}\cap A_1})$ and so $J \subseteq \cap_{i=1}^k \text{Ideal}(\mathcal{C}_{\mathcal{M}\cap A_i}) = \text{Ideal}(\mathcal{C}_\mathcal{M})$.

To prove the converse inclusion, we argue as follows. All the points of $\mathcal{C}_\mathcal{M}$ but $(1:0:\ldots:0)$, $(0:1:0:\ldots:0)$, $(0:1:\ldots:1)$, $(1:0:1:\ldots:1)$, $(k+2:1:\ldots:1)$, $(1:k+2:1:\ldots:1)$ belong to the hyperplane $x_1 - x_2$. The ideal defining those six points can be computed as $\text{Ideal}(\mathcal{C}_\mathcal{M}) : \langle x_1 - x_2\rangle$ (for the colon ideal see (Cox et al., 1997, Ch4.§4)). On the other hand, a direct computation shows that it is equal to $\langle x_l - x_j, (x_1 - x_k)(x_2 - x_k), x_1x_2(x_1 + x_2 - (k+2)x_k) : 3 \leq l < j \leq k\rangle$. Again by direct computation from the generators of J we have

$$J : (x_1 - x_2) = \langle x_l - x_j, (x_1 - x_k)(x_2 - x_k), x_1x_2(x_1 + x_2 - (k+2)x_k) : 3 \leq l < j \leq k\rangle$$

Thus we have that J defines the same set of points outside of $\mathrm{V}(x_1 - x_2)$.

Analogous computation proves that $\text{Ideal}(\mathcal{C}_\mathcal{M}) : (x_l - x_j) = J : (x_l - x_j)$ for all $l \neq j$. Thus $\text{Ideal}(\mathcal{C}_\mathcal{M})$ and J define the same subset of points outside of the hyperplane $\mathrm{V}(x_l - x_J)$. The only point of $\mathcal{M}$ which belongs to all hyperplanes $x_l - x_j$ is the centroid $(1 : \ldots : 1)$. But if we make invertible all polynomials not in $I_C = \langle x_1 - x_k, \dots, x_{k-1} - x_k\rangle$ we see that $J^E + \langle x_1 - x_k, \dots, x_{k-1} - x_k\rangle$ because of the f_{rs} polynomials and so J and $\text{Ideal}(\mathcal{C}_\mathcal{M})$ define the same set in $\mathbb{P}^{k-1}$, i.e. $J = \text{Ideal}(\mathcal{C}_\mathcal{M})$. ■

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